CCSI²

Carbon Capture Simulation for Industry Impact

EPRI – EEMPA Solvent Pilot

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National Energy Technology Laboratory (NETL)

Advanced PSE+ Stakeholder Summit – CCSI² Breakout

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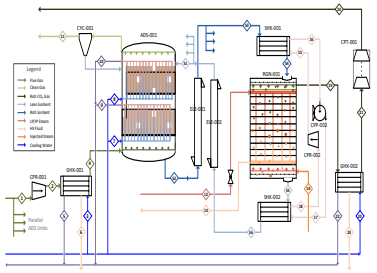
CCSI² – Modeling, Optimization and Technical Risk Reduction

CCSI² Carbon Capture Simulation for Industry Impact

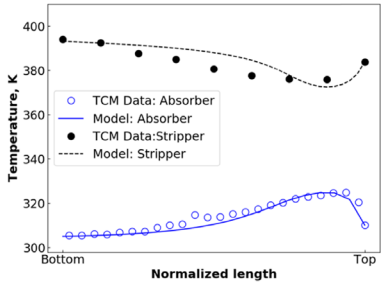
Multi-lab modeling initiative to support carbon capture technology development

National Energy Technology Laboratory · Berkeley Lab · Lawrence Livermore National Laboratory · Los Alamos National Laboratory · Pacific Northwest National Laboratory · Oak Ridge National Laboratory · Carnegie Mellon · West Virginia University · University of Notre Dame · The University of Texas at Austin · University of Pittsburgh

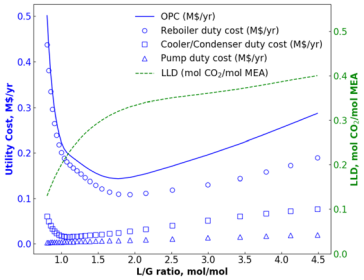
High Fidelity Process Modeling



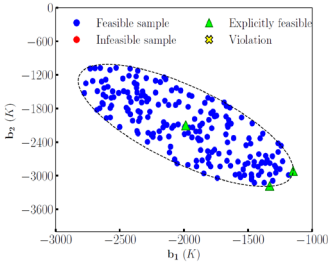
Model Validation



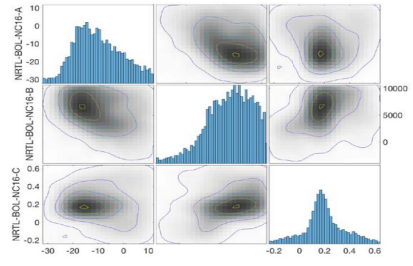
Process Optimization



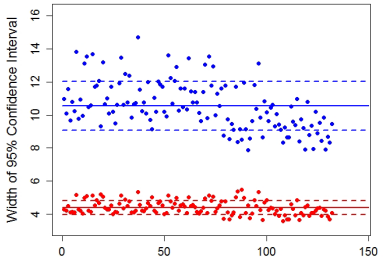
Robust Design

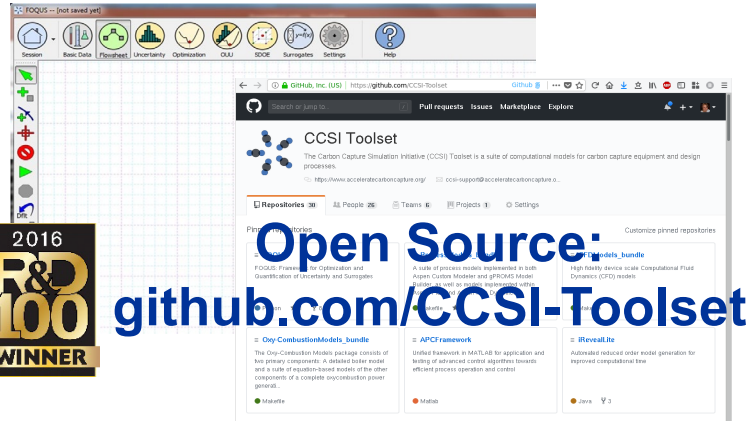


Uncertainty Quantification



Maximizing Learning





2016 R&D 100 WINNER

Open Source:
github.com/CCSI-Toolset

IDAES Institute for the Design of Advanced Energy Systems

Open Source:
github.com/IDAES/idaes-pse

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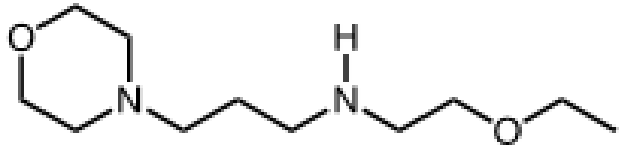
Presentation Overview

- Project Background
- Planning CCSI^2 Support for NCCC Test Campaign
- Current Modeling and Analysis Efforts
- Summary and Conclusions

Project Background – EEMPA Solvent System

- Research team at Pacific Northwest National Laboratory (PNNL) has developed EEMPA solvent system – a promising post-combustion capture solvent



Pacific Northwest
NATIONAL LABORATORY

  - Low viscosity increase associated with CO_2 loading
  - Low corrosivity – potential cost reduction associated with use of less expensive materials in process scale-up (e.g., plastic evaluation)
  - High thermal and chemical stability
  - Reduced heat of absorption → reduced specific reboiler duty (SRD) (< 2.5 MJ/kg CO_2 for optimal operation)
  - Demonstration of 90% capture at lab/bench scale → current modeling efforts suggest higher targets are achievable

Project Background – NCCC Pilot Testing

- Test campaign led by EPRI currently scheduled for 2024 at National Carbon Capture Center (NCCC) (~ 6 month campaign)
- High-level test objectives:
  - Test plastic packing and determine its mass transfer performance
  - Achieve 2 months each on testing coal and natural gas-based flue gases
  - Demonstrate 90% capture on both flue gas types (10 tpd for coal, 5 tpd for natural gas)
- CCSI^2 collaborating with EPRI and PNNL to provide computational support for test campaign – primarily through sequential design of experiments (SDoE) and uncertainty quantification (UQ) work

NATIONAL CARBON CAPTURE CENTER

EPRI ELECTRIC POWER RESEARCH INSTITUTE

Plan for CCSI² Contributions to Support of EEMPA Campaign

Initial Phase
- Plant start-up
- Achieve steady-state water loading

Phase 1
- Demonstrate 90% CO_2 capture for coal, natural gas flue gases
- Use designed experiments to strategically manipulate chosen variables (e.g., solvent circulation, stripper temperature)

Additional Phases
- Target high capture
- Minimize solvent regeneration energy
- Evaluate effect of solvent water content on CO_2 capture
- Investigate effect of flue gas flowrate and temperature
- Analysis of metal vs. plastic packing

Sequential design of experiments (SDoE) enables direct incorporation of knowledge learned in previous stages for strategic data collection

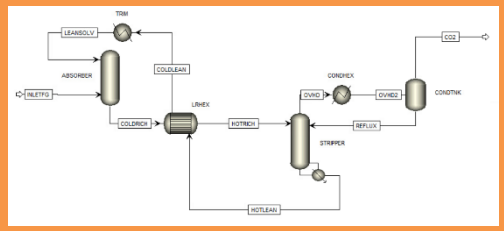
Process Model Refinement

Process Inputs

Solvent Circulation
Solvent Capacity
CO_2 Capture Target
Operating T, P

Model Parameters

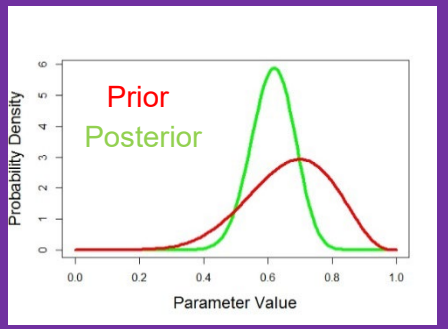
Thermodynamics
Mass Transfer
Interfacial Area
Kinetics



Process Outputs

CO_2 Capture
Specific Reboiler Duty

Stochastic Model
- Reduce risk associated with process scale-up



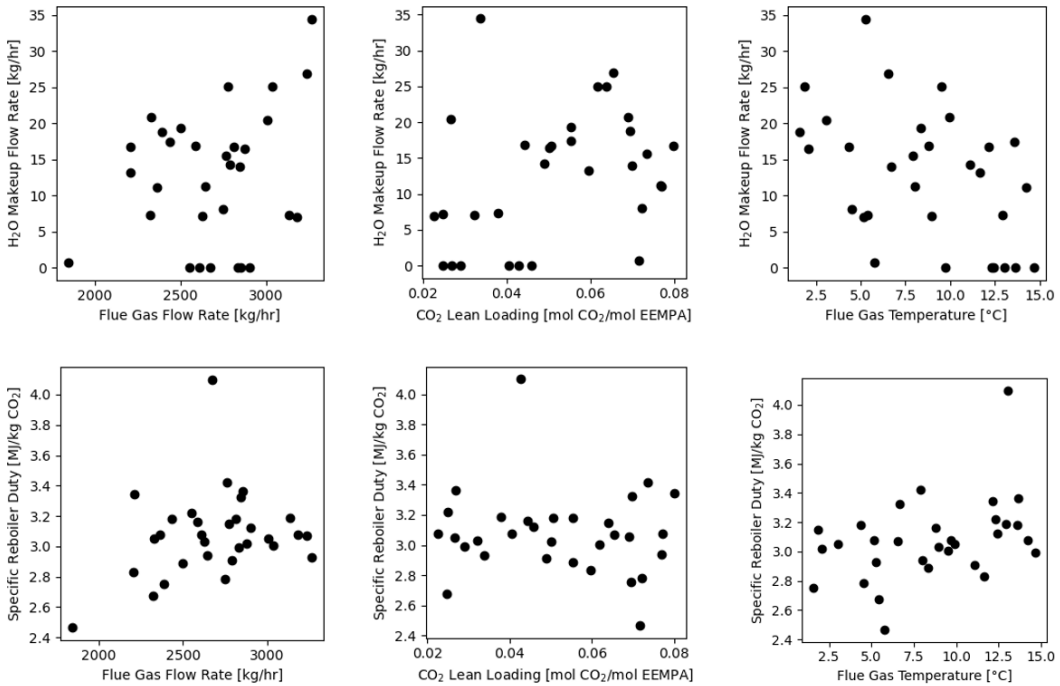
CCSI² Carbon Capture Simulation for Industry Impact

Process Modeling

- Flowsheets developed for NCCC pilot for EEMPA solvent with both coal and natural gas flue gas sources
- Efforts ongoing to identify feasible regions of operation and conduct robustness tests:

Evaluation of NGCC flue gas model over 6-dimensional input space with 100 sample points (90% capture):

- CO_2 Lean Loading
- Flue Gas Flowrate
- Flue Gas Temperature
- Water Concentration in Lean Solvent
- Lean Solvent Temperature
- Stripper Pressure



Model convergence rate around 30% → implies potential for improvement in model robustness

Work ongoing to distinguish between infeasible points vs. failures due to model robustness issues (e.g., convergence hyperparameters, variable initializations, design specification boundaries)

Corresponding analysis for coal-based flue gas is forthcoming

Mass Transfer/Interfacial Area Modeling

Mass Transfer Coefficients (m/s)

Billet & Schultes Model

$$k_{G,ij} = \boldsymbol{C_V} D_{G,ij} \left(\frac{a_p}{d_h}\right)^{\frac{1}{2}} Sc_{G,ij}^{\frac{1}{3}} Re_G^{\frac{3}{4}} \left(\frac{1}{\varepsilon - h_L}\right)^{\frac{1}{2}}$$

$$k_{L,ij} = \boldsymbol{C_L} \left(\frac{g\rho_L}{\mu_L}\right)^{\frac{1}{6}} \left(\frac{D_{L,ij}}{d_h}\right)^{\frac{1}{2}} \left(\frac{u_L}{a_p}\right)^{\frac{1}{3}}$$

Interfacial Area

$$A_I = \left(\frac{a_e}{a_p}\right) a_p \left(\frac{A_c h_c}{N}\right)$$

$$\frac{a_e}{a_p} = \beta_{IntArea}$$

Volumetric Mass Transfer Coefficients (kmol/s)

$$k_{L,ij}^* = k_{L,ij} A_I c_L$$

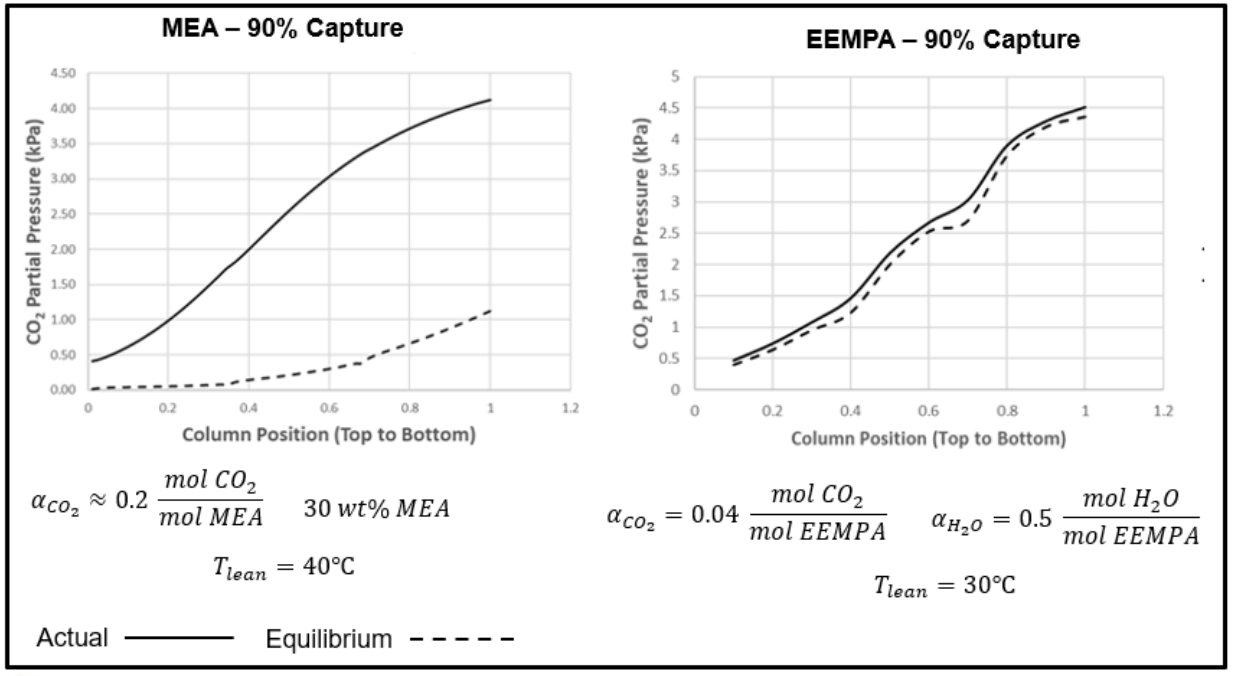
$$k_{G,ij}^* = k_{G,ij} A_I c_G$$

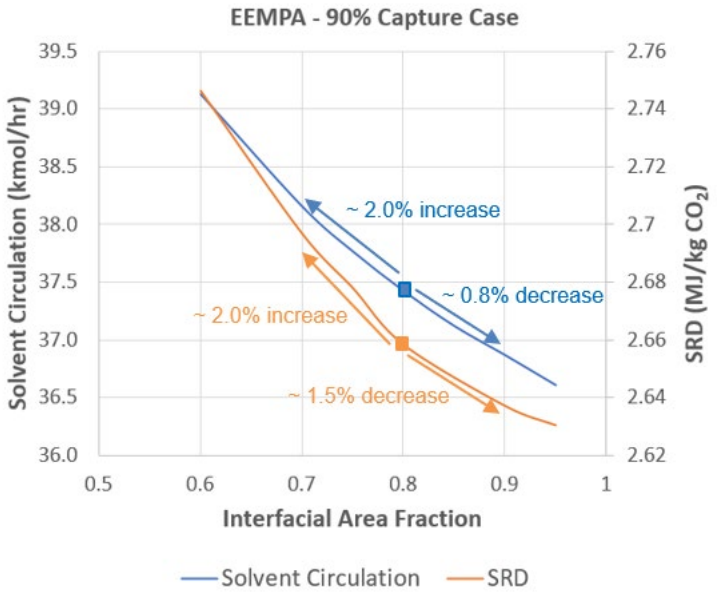
c_L and c_G are molar densities of liquid and gas phases

New interfacial area model being developed by PNNL that is a function of physical properties and can be tuned to different types of packing

Mass Transfer/Interfacial Area (cont.)

- Previous campaigns with MEA solvent focused on reducing parametric uncertainty in mass transfer and interfacial area models under fixed uncertainty in thermodynamic models
  - This method may be less effective for water-lean solvent at 90% capture since performance is projected to be limited by thermodynamics



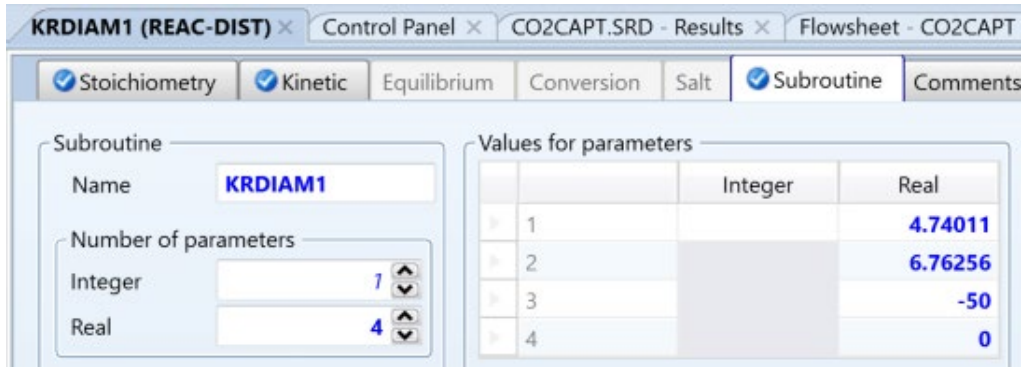


Reaction Kinetics

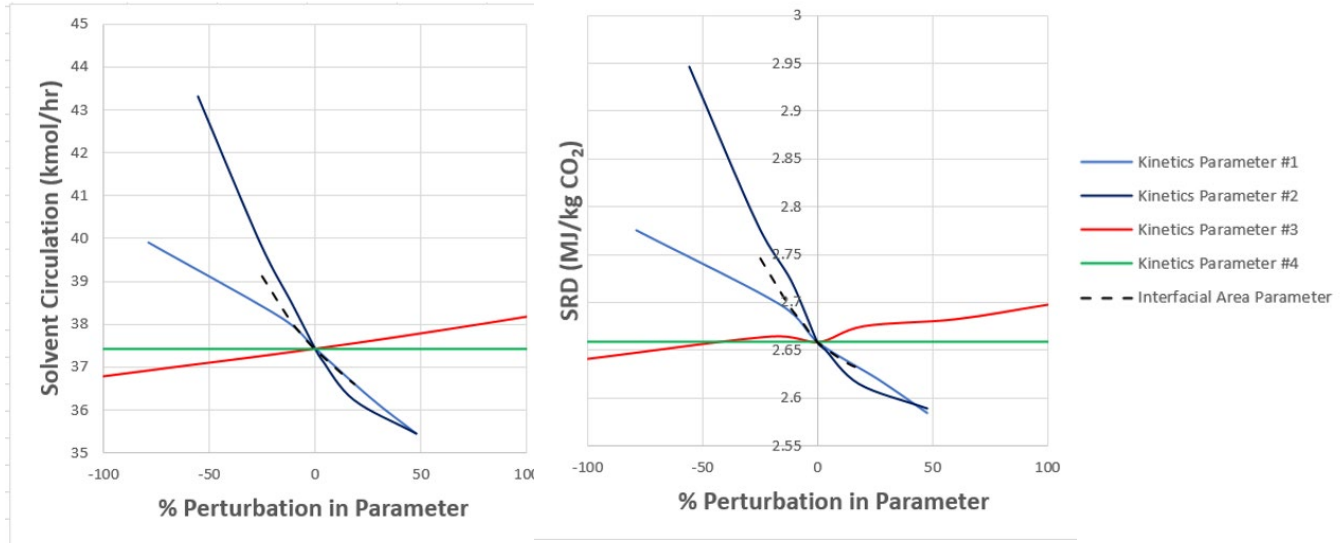
- Essentially a “black-box” model to the CCSI^2 team due to use of user subroutine
  - Four parameters are exposed, can be manipulated in sensitivity analysis/UQ studies

$$2\,DIAM + CO_2 \leftrightarrow DIAMH1^+ + DIAMCOO^- \quad \text{(Rxn 1)}$$

$$DIAM + CO_2 + H_2O \leftrightarrow DIAMH2^+ + HCO_3^- \quad \text{(Rxn 2)}$$



Sensitivity Analysis for Single Input Condition (90% Capture Case)



Thermodynamic Modeling and UQ Analysis

Vapor Liquid Equilibria

$$\hat{f}_i^v = \hat{f}_i^L$$

$$\varphi_i^v y_i P = \varphi_i^L x_i P$$

$$\varphi_i^L = \begin{cases} \frac{h_j \gamma_j^*}{P}; & i = CO_2 \\ \frac{P_i^* \gamma_i}{P} * \phi_i * \varphi_i^v(T, P_i^*) * \delta_i; & i \neq CO_2 \end{cases}$$

This portion generally ≈ 1

Chemical Equilibria

Carbamate formation reaction (j=1):

$$2\ DIAM + CO_2 \leftrightarrow DIAMH1^+ + DIAMCOO^-$$

Bicarbonate formation reaction (j=2):

$$DIAM + CO_2 + H_2O \leftrightarrow DIAMH2^+ + HCO_3^-$$

Temperature correlations used for equilibrium constants (*):

$$K_{eq,j}(T) = A_j + \frac{B_j}{T} = \prod a_i^{\nu_{i,j}} \qquad a_i = \begin{cases} x_i \gamma_i; & i \neq CO_2 \\ x_i \gamma_i^*; & i = CO_2 \end{cases}$$

- Deterministic model developed by PNNL using e-NRTL model implemented in Aspen Plus
- CCSI² using this as a baseline for developing a stochastic model (with parametric UQ)

Thermodynamic Modeling and UQ Analysis

Two sub-systems of interest:

Dry system (EEMPA-CO_2)

$$\left[P_{CO_2}, P_{Amine}\right] = f\left(T, \alpha_{CO_2} \middle| \tilde{\theta}\right)$$

Wet system (EEMPA-CO_2)

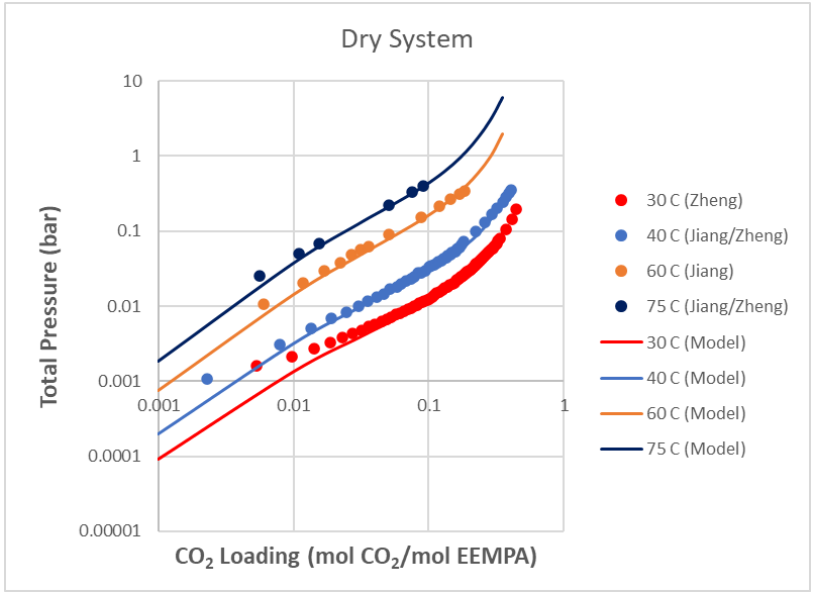
$$\left[P_{CO_2}, P_{Amine}, P_{H_2O}\right] = f\left(T, \alpha_{CO_2}, \alpha_{H_2O} \middle| \tilde{\theta}\right)$$

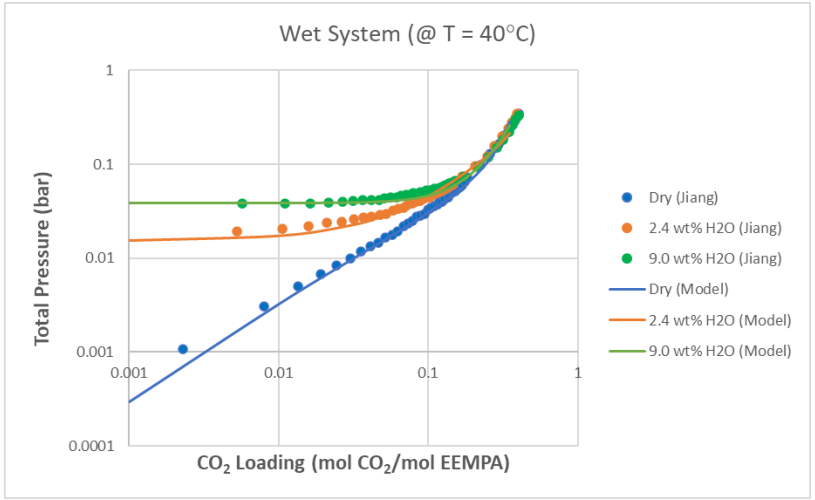
$$P = \sum P_i = P_{CO_2} + P_{Amine} \approx P_{CO_2}$$

Candidate parameters included in set ($\tilde{\theta}$):

i	Definition	Base Value (μ_i)	i	Definition	Base Value (μ_i)
1	NRTL/1 (CO_2/DIAM)	-0.82613	9	GMENCC (DIAM/DIAMH1+,DIAMCOO-)	6.441135
2	NRTL/2 (DIAM/CO_2)	-0.82613	10	GMENCC (DIAMH1+,DIAMCOO-/DIAM)	-3.248471
3	GMENCC (H2O/DIAMH1+,DIAMCOO-)	5.641717	11	GMENCC (DIAM/DIAMH2+,DIAMCOO-)	6.420713
4	GMENCC (DIAMH1+,DIAMCOO-/H2O)	-2.779086	12	GMENCC (DIAMH2+,DIAMCOO-/DIAM)	-3.278853
5	GMENCC (H2O/DIAMH2+,HCO3-)	9.68055	13	Reaction Equilibrium Parameter: A_1	-24.505391
6	GMENCC (DIAMH2+,HCO3-/H2O)	-4.19023	14	Reaction Equilibrium Parameter: B_1	9683.17374
7	GMENCC (H2O/DIAMH2+,DIAMCOO-)	4.620943	15	Reaction Equilibrium Parameter: A_2	-8.959766
8	GMENCC (DIAMH2+,DIAMCOO-/H2O)	-2.379594	16	Reaction Equilibrium Parameter: B_2	4000

Activity Coefficient Parameters Chemical Equilibria Parameters





Data sources:
Jiang et al., *Int. J. Greenh. Gas Con*. 106: 103279.
Zheng et al., *Energy Environ. Sci*. 13: 4106.

Additional unpublished data sets used to develop model for wet system:
~ 40°C (2 wt% H_2O, 5 wt% H_2O)
~ 65°C (2 wt% H_2O)

Thermodynamic Modeling and UQ Analysis

Formulation of Prior Distribution:

$$P(\theta_i) \sim N(\mu = \mu_i, \sigma^2 = \left(\mu_i \frac{\alpha_i}{3}\right)^2)$$

$\alpha_i = 0.2$ Activity Coefficient Parameters

$\alpha_i = 0.05$ Chemical Equilibria Parameters

α_i is defined as an uncertainty level
(e.g., $\alpha_i = 0.2$ implies a 99.7% prediction interval for parameter θ_i that is ± 20% of $|\mu_i|$)

Surrogate Model Development and Validation:

Model developed from an input/output sample generated from Aspen Plus ($n = 1000$) (*):

$T \sim U(20,90)$ [°C]

$\alpha_{CO_2} \sim U(0,1)$ [mol CO_2/mol Amine] (*)

$\alpha_{H_2O} = 10^{-5}$ [mol H_2O/mol Amine] (**)

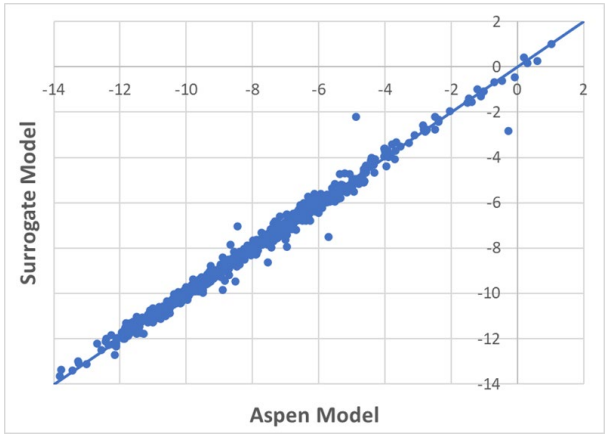
$\theta \sim P(\tilde{\theta})$ (specified prior distribution)

(*) Range too wide – resulted in some failures in the simulation ensemble → $n = 770$ converged runs ultimately used for development of surrogate model

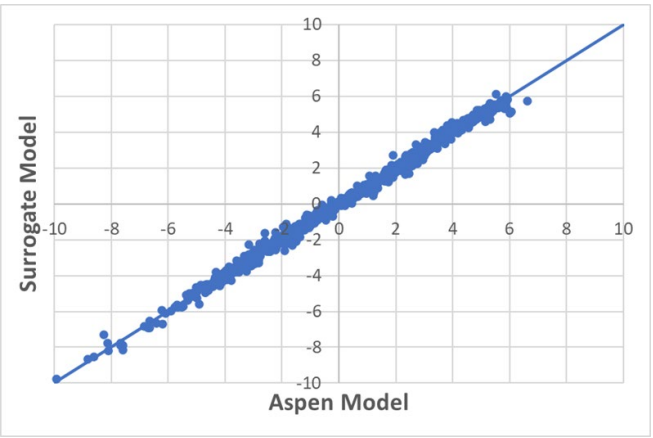
(**) Dry system – trace amount of H_2O used to avoid computational error

Surrogates developed independently (using same input sample):

$\ln(P_{Amine}[bar])$

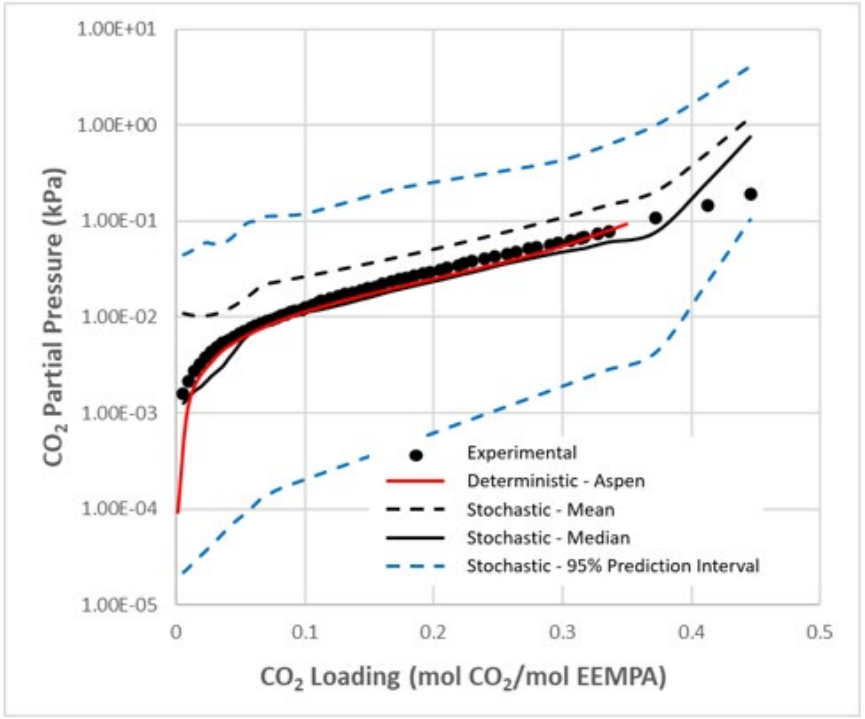


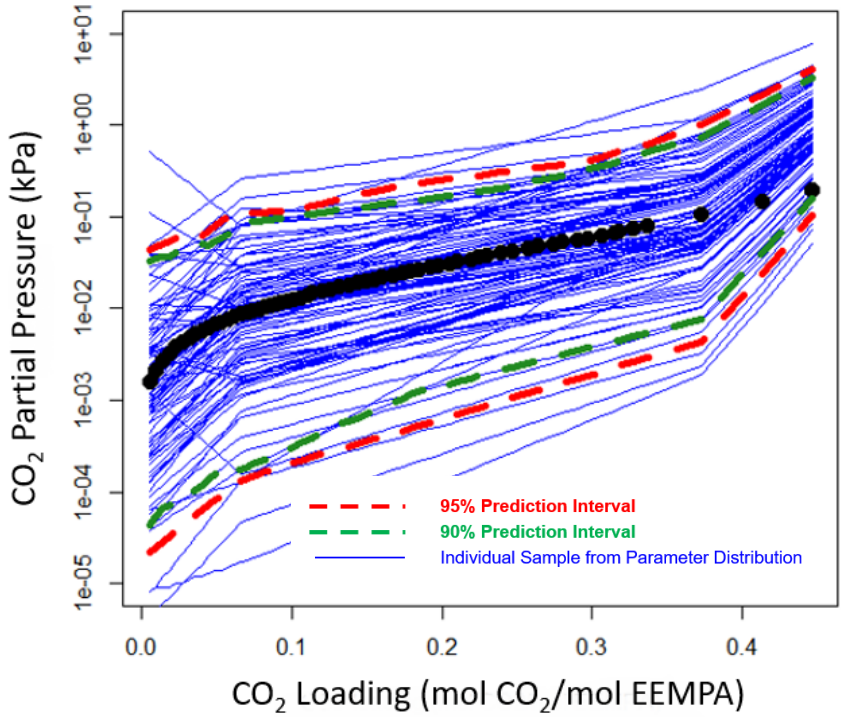
$\ln(P_{CO_2}[bar])$



Thermodynamic Modeling and UQ Analysis

Evaluation of stochastic surrogate model for dry system (@ 30°C):



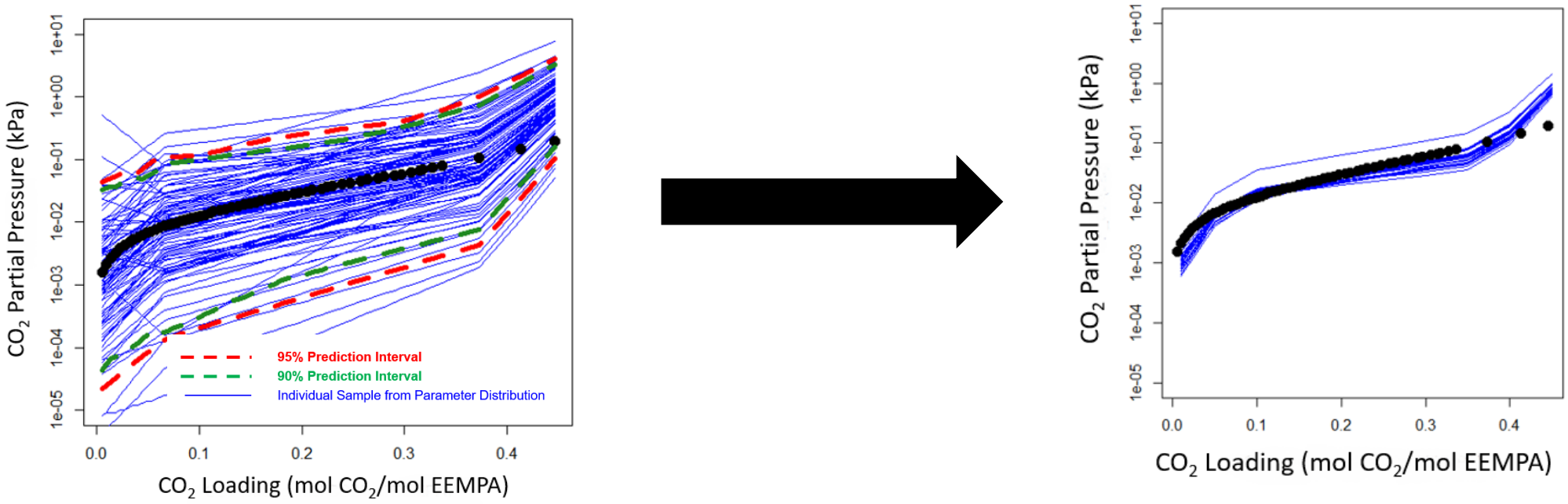


Specified prior distribution result in predictions of VLE that are too broad:

- Good starting point for refining parameter estimates
- Bayesian inference provides platform for incorporating experimental data for refining parameter distribution → can characterize parameter ranges and interactions
- Bayesian inference requires assumption on uncertainties in experimental data

Thermodynamic Modeling and UQ Analysis

Effect of Bayesian inference – preliminary results



- Algorithm produced a posterior with $n = 50000$ realizations of $\tilde{\theta}$; only 26 were unique
- Future efforts will focus on identification of best practices for characterizing

Summary and Conclusions

- CCSI^2 team planning computational support for pilot campaign for EEMPA solvent at NCCC in 2024
- Current process modeling efforts focused on:
  - Identifying feasible operating regions for process with natural gas and coal-based flue gas sources
  - Formulating UQ problems for process submodels – thermodynamics, reaction kinetics, mass transfer/interfacial area
- Challenges being addressed:
  - Identifying best practices for UQ – prior distribution formulation, ensuring sufficient accuracy of surrogate models for Bayesian inference
  - Analyzing and improving model robustness over a range of operating conditions and levels of CO_2 capture

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Disclaimer

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Carbon Capture Simulation for Industry Impact

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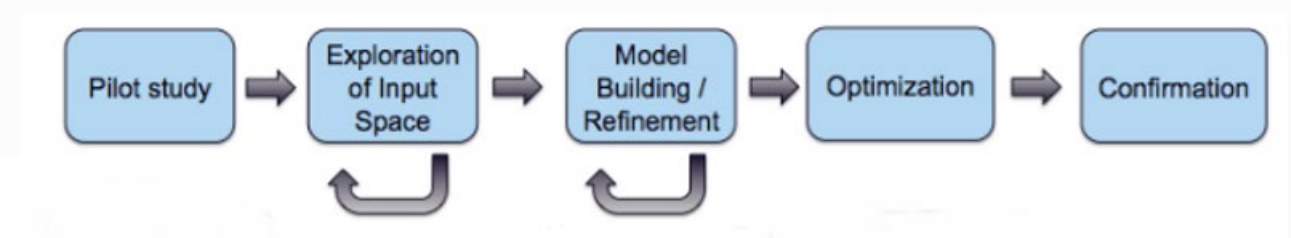
Backup Slides

Sequential Design of Experiments (SDoE)

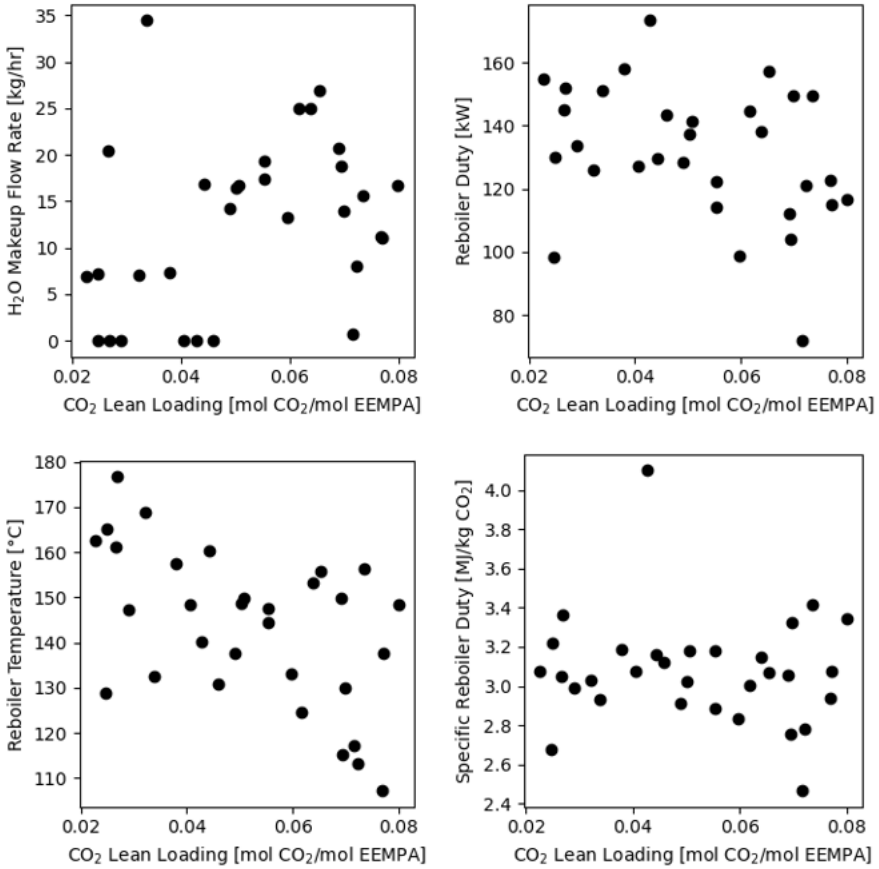
- **Design of experiments (DOE)** is a powerful tool for accelerating learning by targeting maximally useful input combinations to match experiment goals
- **Sequential design of experiments (SDoE)** allows for incorporation of information from an experiment as it is being run, by updating selection criteria based on new information
- Specific algorithms can be tailored to match experimental goals. Options available in the CCSI Toolset include:
  - Uniform Space Filling (USF)
  - Non-Uniform Space Filling (NUSF)
  - Input-Response Space Filling (IRSF)
  - Robust Optimality-Based Design of Experiments (ODoE)
- Recommended to run experiments in phases to take advantage of SDoE capabilities and customize test designs to meet expected project outcomes



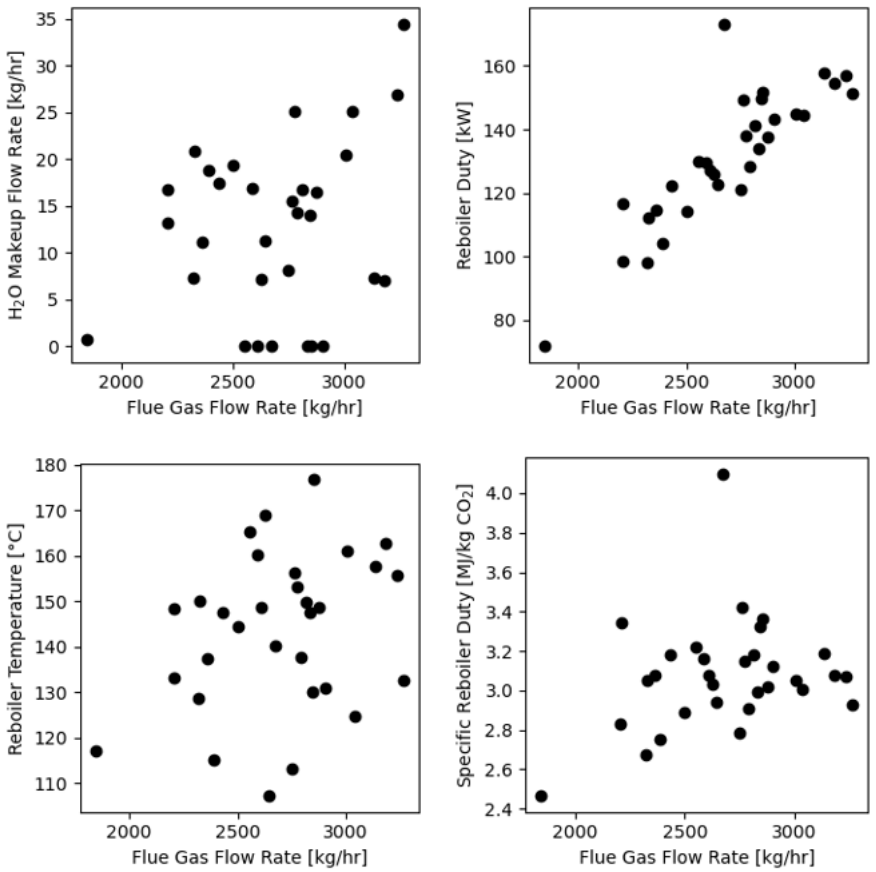
Detailed discussion on SDoE:

NCCC NGCC EEMPA Model – Robustness Tests

CO_2 Lean Loading



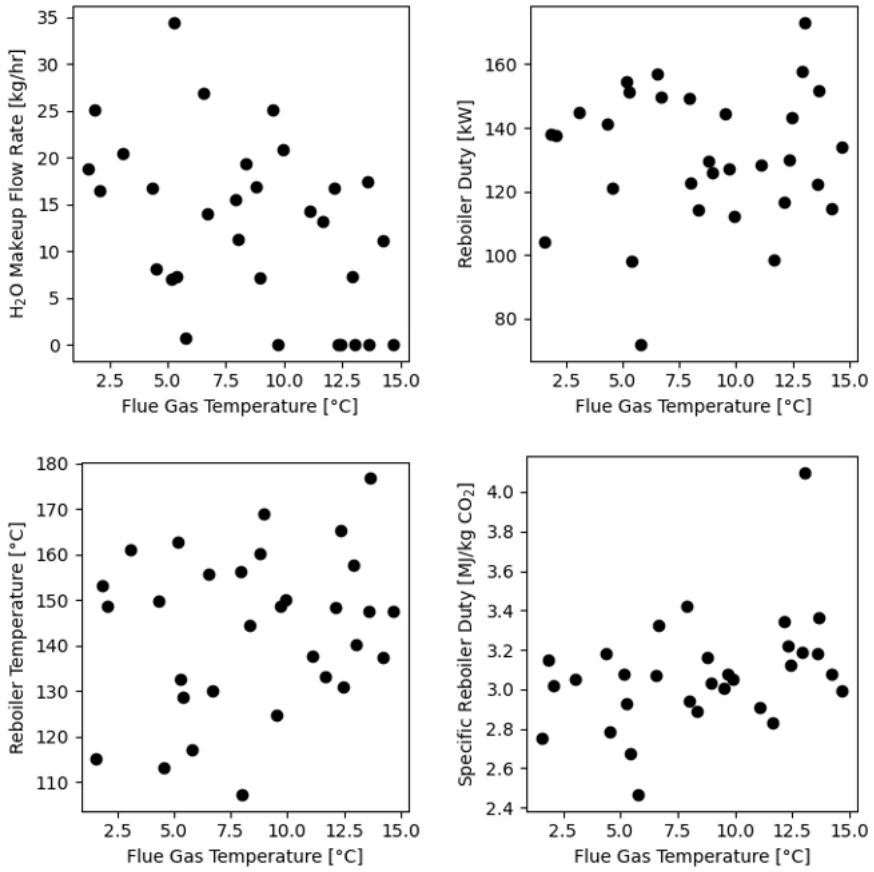
Flue Gas Flow Rate



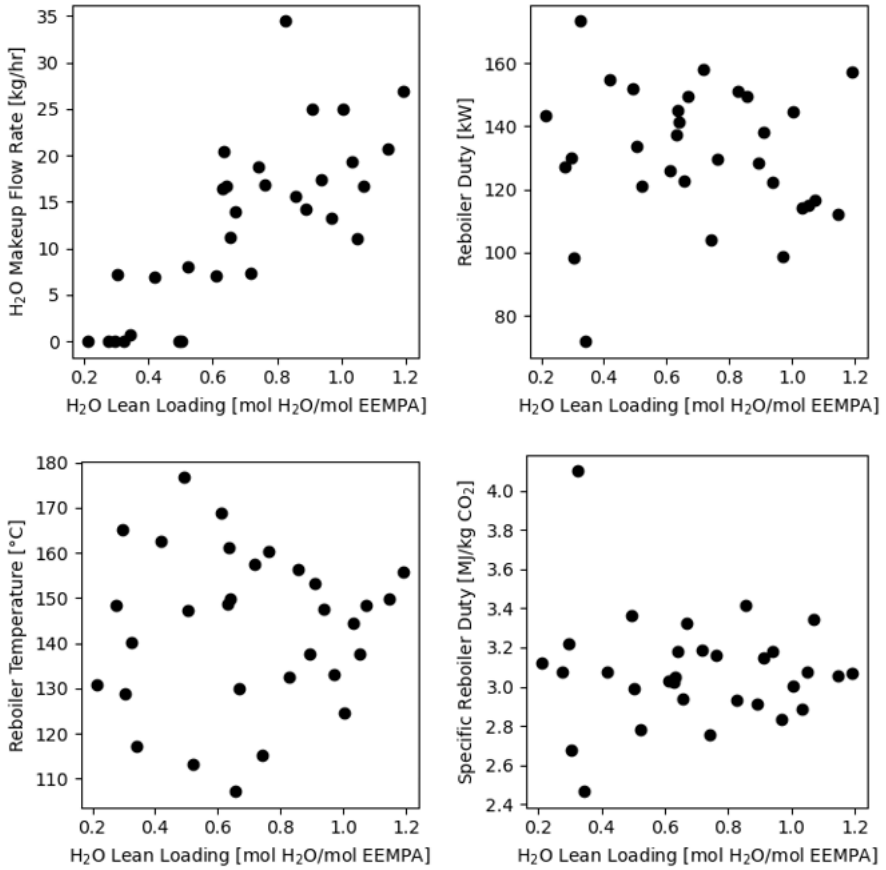
● Denotes converged simulation

NCCC NGCC EEMPA Model – Robustness Tests

Flue Gas Temperature



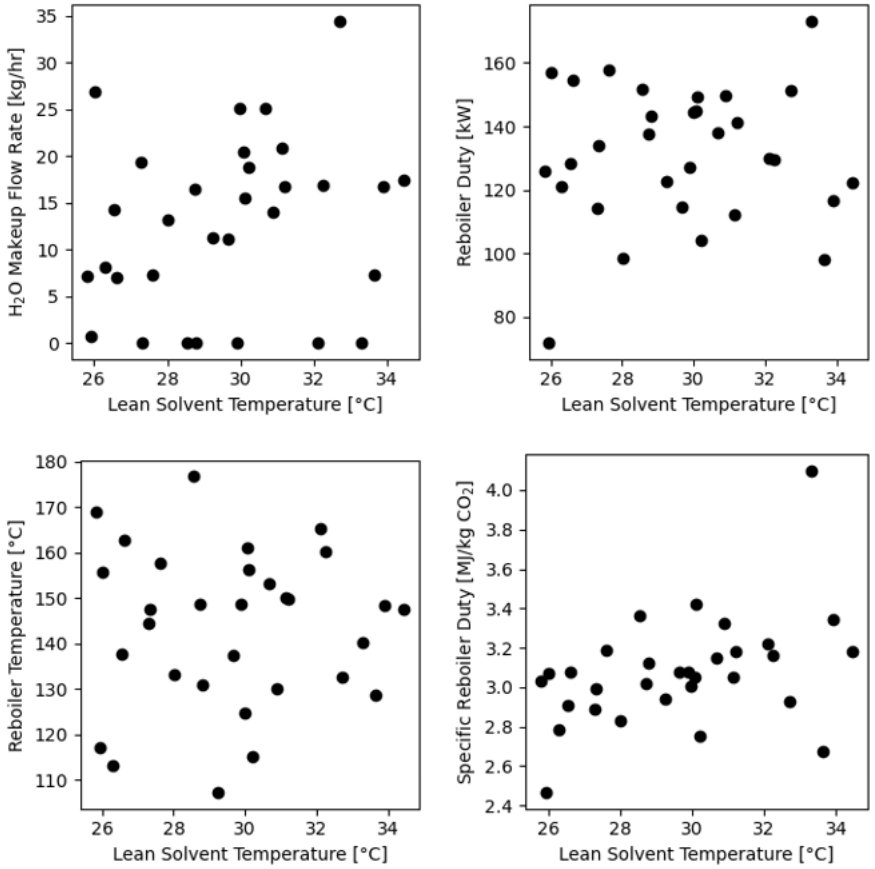
H_2O Lean Loading



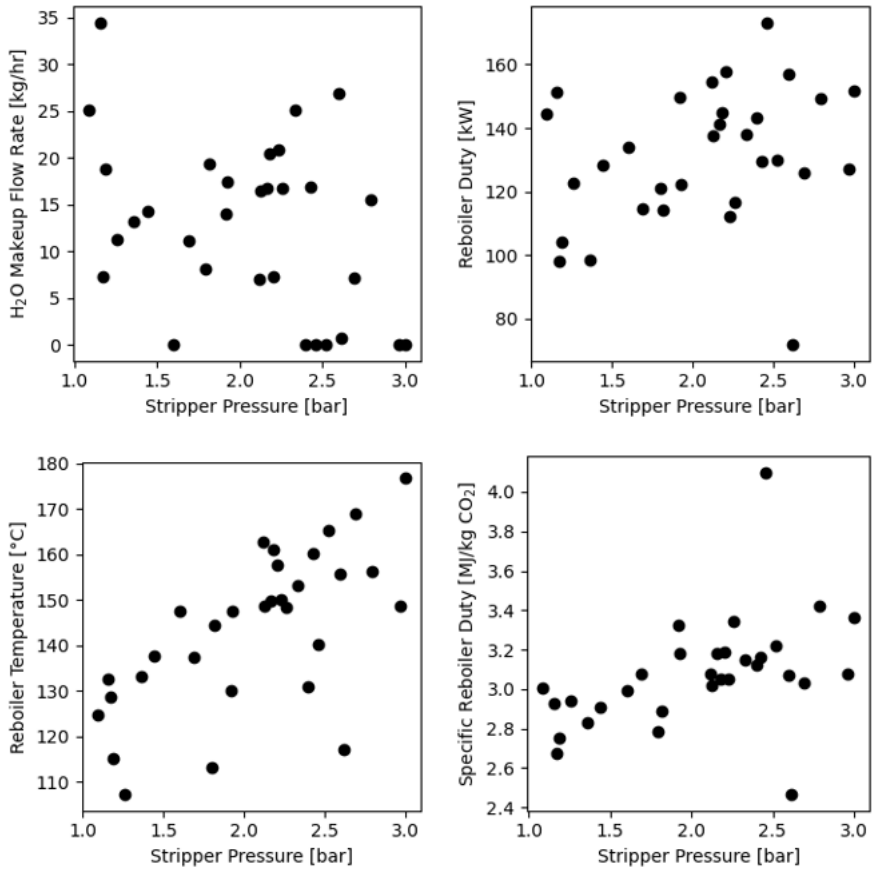
● Denotes converged simulation

NCCC NGCC EEMPA Model – Robustness Tests

Lean Solvent Temperature



Stripper Pressure



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