Model-Based Sequential Design of Experiments for Pilot Testing of Novel Water-Lean CO_2 Capture Solvent

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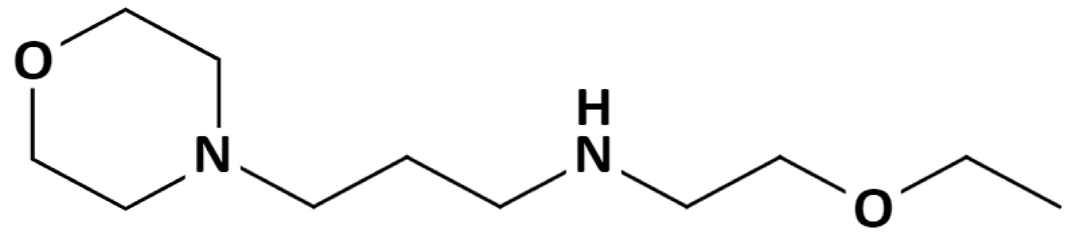
EEMPA

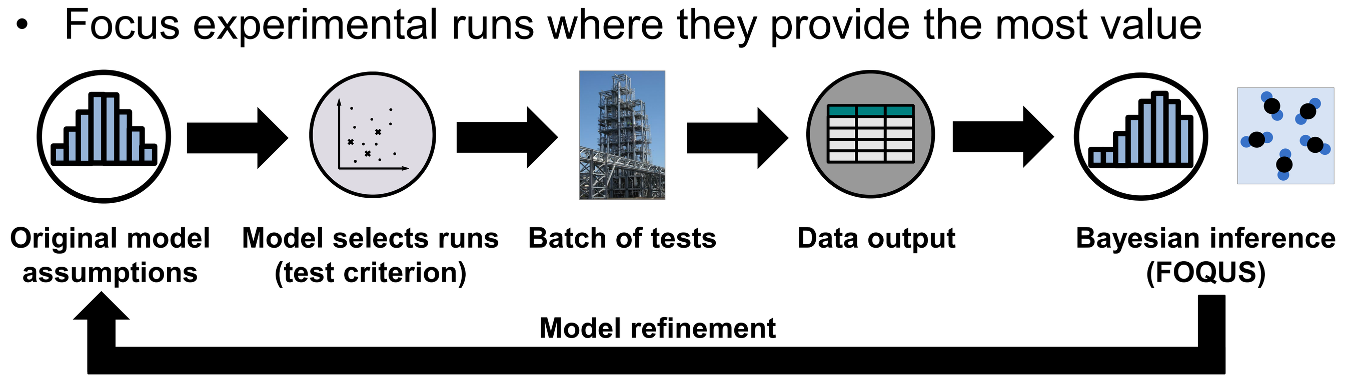
- N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (EEMPA) is a CO_2 binding organic liquid (CO_2BOL)—a type of water-lean solvent developed by Pacific Northwest National Laboratory[1]



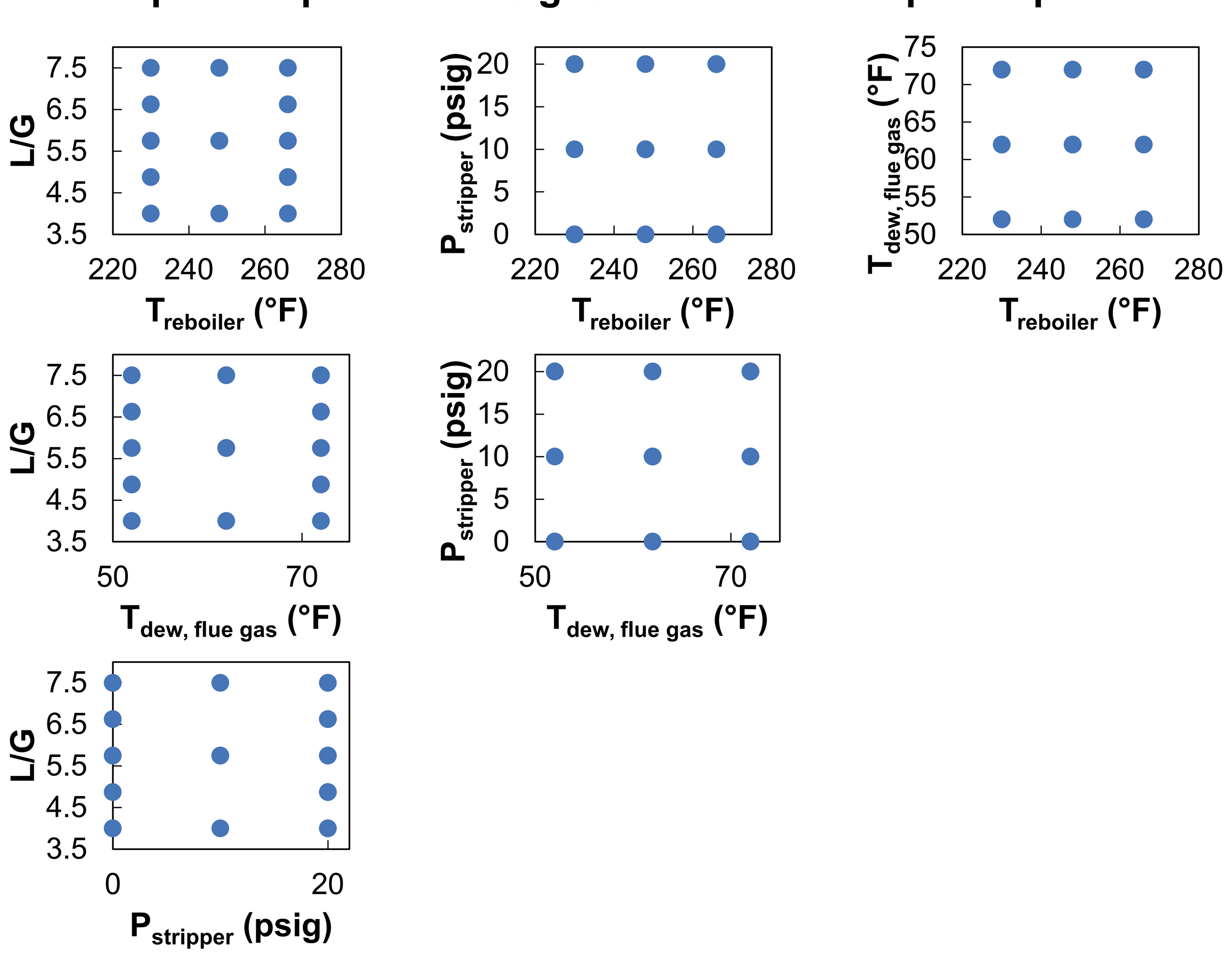
- Using CO_2BOLs compared to monoethanolamine (MEA) allows:
  - Reduced reboiler duty
    - Lower reboiler temperature
    - Lower vaporization duty
  - Reduced degradation
  - Reduced CO_2 compression costs—increased regeneration pressure
  - Ability to use plastic packing

Sequential Design of Experiments (SDoE)

- Utilize data from experimental runs to inform choice of future sample points to reduce uncertainty, refine model parameters, etc.
- Focus experimental runs where they provide the most value

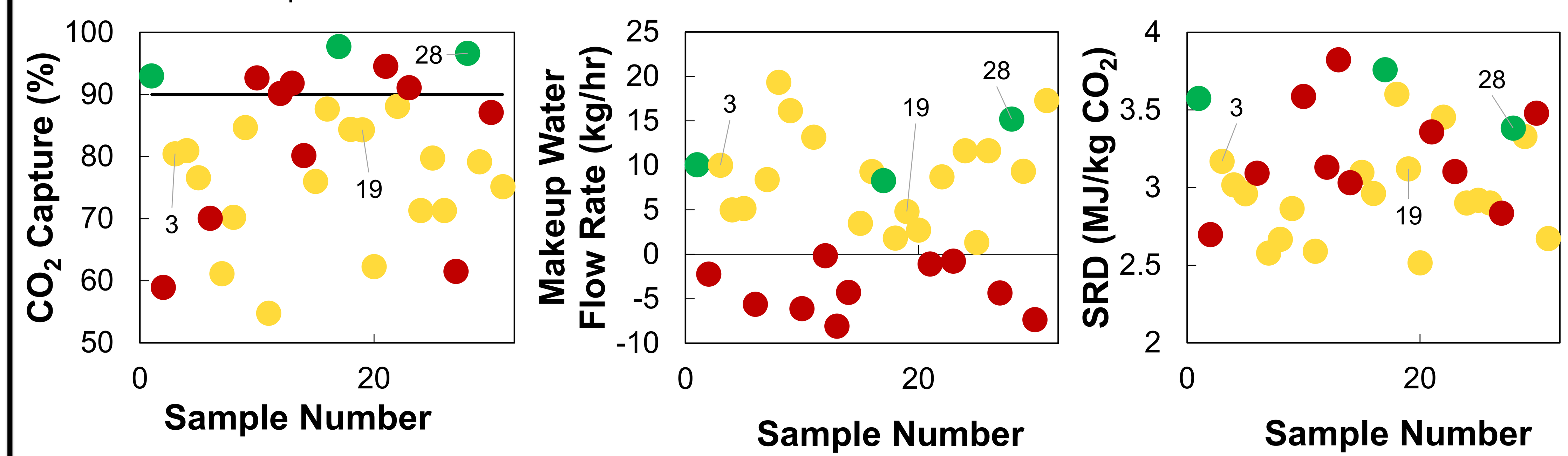


- **Example test plan for flue gas from coal-fired power plant:**

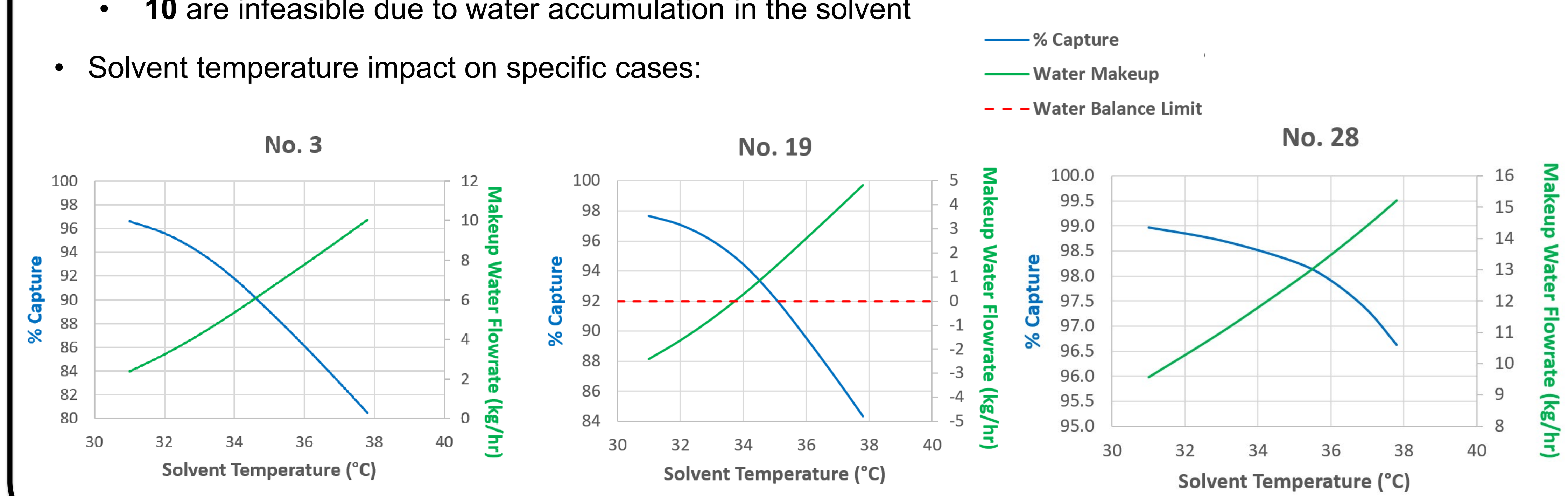


Process Modeling

- Model set up to simulate EEMPA-based carbon capture system for flue gas from coal-fired power plant
- **Using inputs from SDoE example test plan** – 31 samples
  - **Constant solvent temperature (37.8°C)** – opportunity to increase capture by decreasing solvent temperature



- Out of 31 samples
  - **3** meet the desired criteria of high capture (above 90%) while maintaining the water balance
  - **18** (additionally) maintain the water balance
  - **10** are infeasible due to water accumulation in the solvent
- Solvent temperature impact on specific cases:



Test Campaign Goals and Plan

- Test two flue gases: NGCC and coal-fired power plant flue gas
- Establish water balance—limited to 10 wt% of solvent
- Establish operating conditions necessary to achieve 90% capture
- Use SDoE to quantify model uncertainty and refine process conditions to achieve greater than 90% capture at optimized reboiler duties
  - Implement test plan developed with contributions from modeling insights
  - Update model based on initial samples using Bayesian Inference
  - Develop new test plan using SDoE
  - Implement new test plan and repeat as time allows
- Demonstrate long-term operability of the solvent at optimized conditions
- Test performance impact of plastic packing

Uncertainty Quantification

- 16 thermodynamic parameters: 12 binary interaction parameters and 4 reaction equilibrium parameters
- Using Bayesian Inference

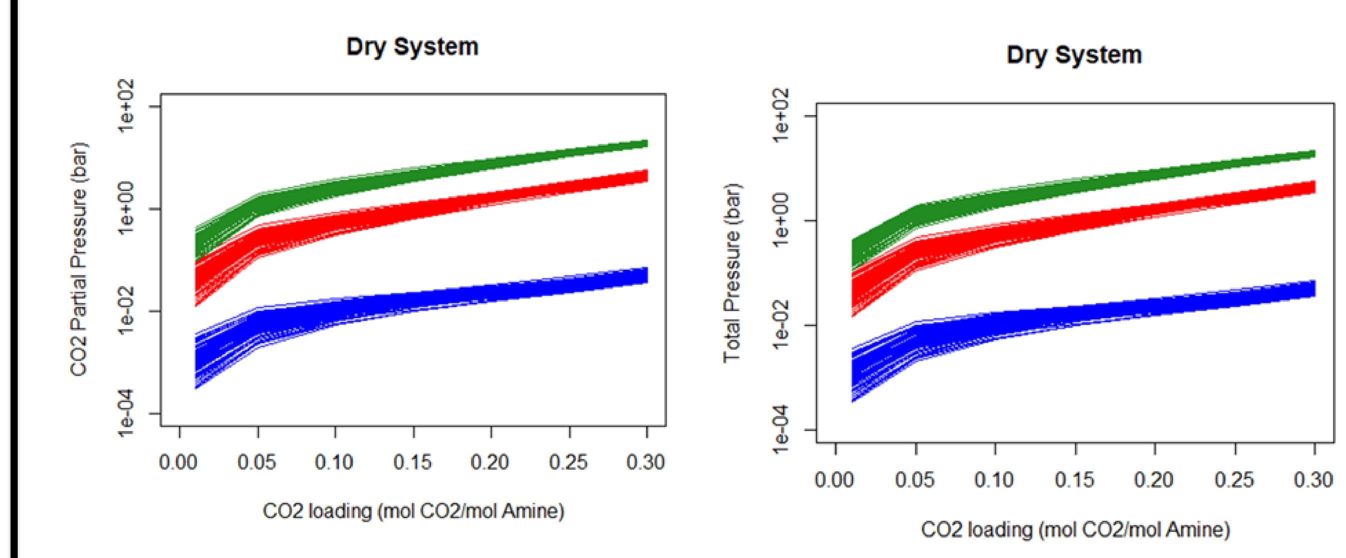
$$P(\theta_i|Z) = \frac{P(Z|\theta_i)P(\theta_i)}{P(Z)} \propto P(Z|\theta_i)P(\theta_i)$$

- Prior distribution

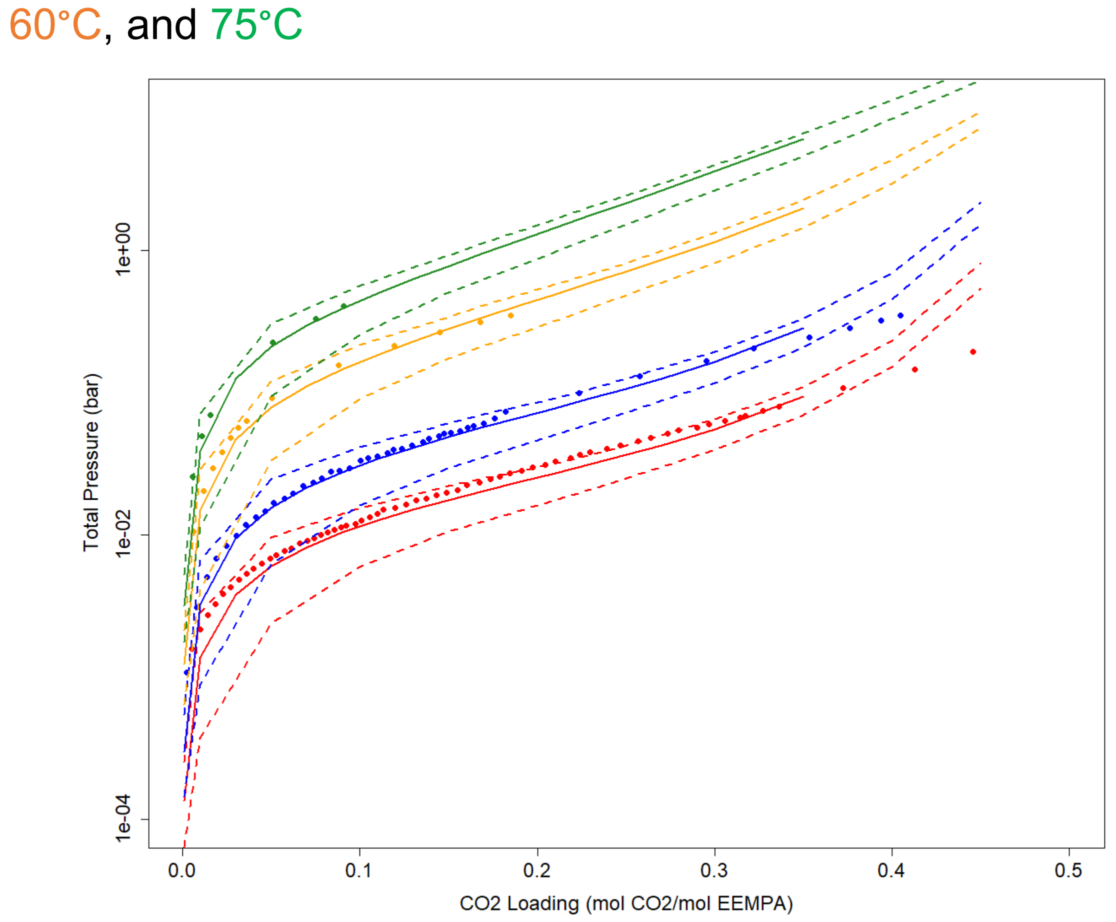
$$P(\theta_i) \sim N\left(\mu = \mu_i, \sigma^2 = \left(\mu_i \frac{\alpha_i}{3}\right)^2\right)$$

where the chosen value of α_i is 0.2 for parameters 1–12 and 0.05 for parameters 13–16

- Posterior propagated through VLE model for temperatures of 30°C, 80°C, and 120°C



- Comparison to experimental data at temperatures of 30°C, 40°C, 60°C, and 75°C



References

[1] Jiang Y. et al., 2023. Energy-effective and low-cost carbon capture from point-sources enabled by water-lean solvents. Journal of Cleaner Production. Volume 388.

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CCSI2 Carbon Capture Simulation for Industry Impact

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