Bayesian parameter estimation for the model development of the water lean amine solvent CO_2 capture process

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The accurate evaluation of KHU-B, which is the water lean amine solvent and developed by our research team, is impossible without the development of the process model. Inaccuracy in experimental results and the incomplete knowledge of model parameters are problems which have a crucial effect on the reliability of process models.

Here, we solve their uncertainty problems and develop the CO_2 capture process model for KHU-B. To detect non-influential parameters and their interactions (parameter subset selection), we carry out the global sensitivity analysis using Sobol' indices in CO_2 capture model of ASPEN plus. After that, we make the quadratic hyper-surface surrogate model which reflects the interaction between selected parameters. The calibration of the proposed model using experimental data is conducted to estimate the parameters from Bayesian inference using Markov Chain Monte Carlo (MCMC) with Metropolis-Hastings algorithm.