Validation and Uncertainty Quantification of a High-Fidelity Dynamic Model of a MEA-Based CO_2 Capture System

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With growing concern over global CO_2 emissions, it is essential that efficient post-combustion CO_2 capture technologies are developed and deployed. The U.S. Department of Energy's *Carbon Capture Simulation Initiative* (CCSI) is focused on developing computational tools and models to accelerate the development and commercialization of post-combustion CO_2 capture technologies. The process modeling team of CCSI is developing high-fidelity process models which can be used by the industry to rapidly design and scale up such processes while also improving their operability. However, uncertainty in properties and process models can significantly affect the predictability of these models. In addition, the model should be validated with the experimental data in the expected region of operation. With this incentive, a high-fidelity dynamic model of a monoethanolamine (MEA) based CO_2 capture process is developed. Rigorous uncertainty quantification (UQ) analysis is performed for the key thermodynamic and transport models such as density, viscosity, surface tension, heat capacity, diffusivity, and VLE models. In addition, UQ analysis is performed for the interfacial area, holdup, pressure drop, mass transfer, and heat transfer models. For each model, baseline values of the parameters are first obtained by minimizing the sum of squared error between the model results and the experimental data. The best guess for parametric uncertainty (priors) is then cast in the framework of a Bayesian inference methodology to obtain more informed posterior parametric uncertainty. However, many properties and process models are highly parameterized. The computational expense for using the Bayesian approach to these models can be prohibitive. Therefore, response surface models are generated as computationally inexpensive surrogate models with sufficient accuracy by using the input-output data. The Markov Chain Monte Carlo (MCMC) analysis with Gibbs sampling is applied to the response surface to generate posterior distributions for the parameters by Bayesian inference. Finally, the posterior distributions in all parameters are propagated through the process model to obtain the uncertainty bounds in key operating variables. These results are compared with the data collected from the US DOE's National Carbon Capture Center (NCCC) located in Alabama. The process models are developed both in Aspen Plus and gPROMS platforms. The UQ capabilities in the properties models have been developed in Aspen Properties with user models developed in FORTRAN.

Finally, a dynamic model of this system is developed and validated with the dynamic data from the NCCC. The validation studies and transient results provide valuable insights about the MEA-based CO_2 capture processes under uncertainty.