(707c) Optimal Model Synthesis for Solvent-Based CO2 Capture Systems By Simultaneously Using Multi-Scale Data

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Rigorous process models allow accelerated development of advanced energy systems by reducing the risk and uncertainty in scale up thereby requiring fewer intermediate process scales to be built. It is desired that the sub-models, such as mass transfer and holdup, be scale independent and that they should be able to discriminate and neglect measurement error. Furthermore, it may be difficult to isolate the effect of one mechanism from others if they are fast and take place simultaneously. For example, in chemical solvent-based CO_2 capture systems, such as the MEA-H_2O-CO_2 system, very fast reaction kinetics make it almost impossible to measure the mass transfer flux separately. A typical approach to this problem is to use a surrogate component, such as N_2O, that does not participate in the reactions. Even though such surrogate components may have strong similarity to CO_2, mass transfer characteristics and thermo-hydraulic behavior of the loaded solvent is not

necessarily the same as the CO_2-loaded solvent. The use of a surrogate component also fails to capture the true enhancement of mass transfer due to fast chemical reactions.

Another approach is to carefully design experiments at small scale to identify models which are assumed to be valid at larger scales where additional effects/mechanisms are captured. For example, the diffusivity model is assumed to be a satisfactory mass transfer model for typical chemical solvent-H_2O-CO_2 systems since diffusivity is almost impossible to measure in these systems. Then, mass transfer coefficients are calculated from wetted wall column (WWC) experiments. Experimental data from packed columns are then used to obtain the interfacial area model assuming the mass transfer coefficient models derived from WWC data are valid in the packed column. Because the WWC and packed column operate in different flow and operating regimes, the mass transfer coefficient models and their parameters are not necessarily appropriate (or optimal) for the packed column. In addition, the accuracy of the diffusivity model is questionable.

One way to circumvent the issues discussed above is to perform simultaneous identification of multiple sub-models and parameter estimation by concurrently using experimental data from the packed columns, wetted wall columns, and other laboratory or plant measurements. However, such simultaneous regression is not feasible in existing state-of-the-art simulation software. In this work, a novel modeling and optimization framework is developed in Pyomo to achieve this goal.

First, detailed models of the absorber, regenerator, plate-and-frame heat exchanger for the lean/rich solvent, and stripper reboiler are developed which utilize rigorous models for the thermodynamic and transport properties. The rate-based model of the packed columns include high-fidelity sub-models for the diffusivity, interfacial area, liquid holdup, reaction kinetics, and mass transfer coefficients. In addition, a detailed reboiler model is developed by considering mass and energy balances and a liquid phase speciation model coupled with detailed thermo-physical properties models. A rigorous model of a plate-and-frame heat exchanger is also developed using the effectiveness-number of transfer unit (e-NTU) method.Â The rigorous model is used for simultaneous model synthesis and parameter estimation utilizing data from multiple scales from wetted wall columns to small packed towers to large pilot plants such as the U.S. DOEâ€™s National Carbon Capture Center in Wilsonville, AL. Our work shows that such a framework can be useful for obtaining highly predictiveÂ scale-invariant models .

Abstract:

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