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Process design optimization model for amine scrubbing

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Abstract

An amine scrubbing process model called "Rainier" is implemented in gPROMS Process® as an equation-oriented model using rate-based mass transfer[1]. The purpose of this model is to identify cost-optimal equipment design and steady-state operating conditions for a capture application given a set of conditions or targets for flue gas composition, flow, CO_2 capture rate, etc. Operating and capital costs are estimated as part of the model, allowing for optimization to be done with an objective of minimizing cost of capture in terms of $/tonne of CO_2 captured. Other economic, process, or environmental objectives are also possible.

Equation-oriented optimization models for different capture technologies have shown that this cost optimization approach can be used to identify designs which reduce cost of capture compared to baseline heuristically-designed processes[2-4]. The scope of this work is to simulate capture using aqueous piperazine. The initial basic process configuration is the Piperazine with the Advanced Stripper (PZAS) process as designed for a retrofit of a natural gas combined-cycle (NGCC) power plant[5]. The model uses an apparent species approximation to estimate liquid-phase properties. A thermodynamically consistent set of equations describes thermodynamic properties and is fitted to experimental measurements of the PZ-H_2O-CO_2 equilibrium. The liquid-film mass transfer coefficient (k_g'), a key component of the rate-based mass transfer model, is regressed by a data-driven approach using a previous high-order model of PZAS[6]. This approach makes it possible for future work to extend the model to other solvents given a limited set of data on the properties of the new solvent.

A challenge with this cost optimization task is that capital costs for this type of process are difficult to estimate. Equipment cost estimates for commercial-scale capture processes are often inaccurate in academic studies, and costs associated with retrofitting an existing power plant (or other point source) with capture are difficult to predict[7]. A front-end engineering design (FEED) study was completed for a retrofit of an NGCC, and the study, including cost estimates, was published in the open literature[5]. This FEED study and others provide a realistic baseline for equipment costs and capital costs in commercial-scale capture processes, and comparing these studies provides insight into drivers of cost in retrofit projects[8]. Costs and learnings from the FEED study will serve as the basis of an equipment cost and capital cost estimating module in Rainier.

Absorber model

A model of the CO_2 absorber was previously developed and compared against an existing PZAS model and pilot-scale experiments[6]. The liquid phase is modeled as consisting of three apparent components: PZ, H_2O, and CO_2. This is different from a true species approach, which would model many ionic species resulting from chemical reactions of the three apparent species. The vapor pressure (P_i) of each component is represented by a polynomial function of temperature and solvent loading (α). For thermodynamic consistency, heat of vaporization (ΔH_{vap}^i) and heat capacity (C_p^i) of each component are calculated by the

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appropriate derivatives of the vapor pressure equations[6].

Deficiencies were identified in the accuracy of the thermodynamic properties, particularly the liquid heat capacity. Equilibrium data for PZ in solutions of PZ-H_2O-CO_2 were reviewed[9-12]. There have been a limited number of experimental measurements of ΔH_{vap}^{PZ} or C_p^{PZ} for CO_2-loaded solutions. Figure 1 shows P_{PZ} for various concentrations of PZ at various temperatures as a function of loading. Dashed lines indicate the P_{PZ} correlation used in the model. The fit deviates from the experimental data, especially at lower temperatures (the range relevant to the absorber). Improving the accuracy of the thermodynamic model is an ongoing task. The results presented in this abstract use the correlation by Xu as shown in Figure 1[12].

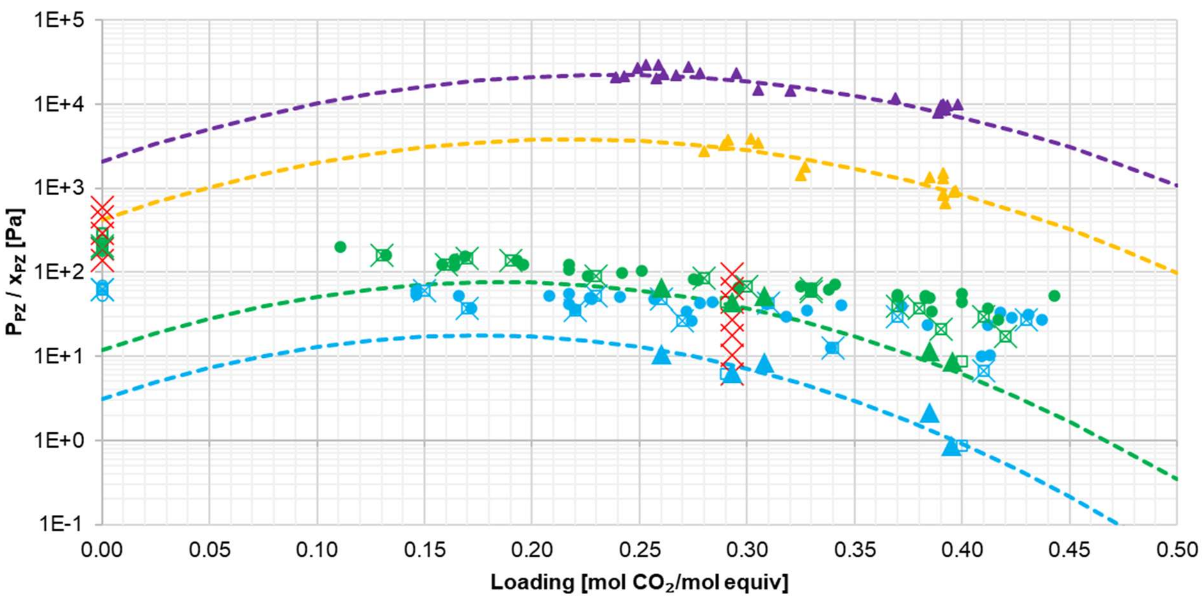

Figure 1: Vapor pressure of PZ normalized by mole fraction of PZ vs. loading. Colors indicate temperature in °C: 40 = blue, 60 = green, 120 = yellow, 150 = purple, various = red. Circles: Hilliard[9], Crosses: Nguyen[10], Squares: Nguyen et al.[11], Triangles: Xu[12]. Curve: Xu[12]

Full-flowsheet model

The intercooled absorber model described above is implemented as a module within a larger model of the full process flowsheet, shown in Figure 2. The EXCHANGERS block contains solvent cross-exchangers for heat integration of the rich and lean solvent and an optional trim cooler. Presently, a simple heat exchanger model is used which does not account for flashing of solvent and which takes a user-specified pressure drop. It is expected that the optimal process design could involve flashing a portion of the rich solvent in the exchanger before it enters the stripper. Pressure drop in the exchangers is a critical variable, because the sizing of the exchangers and the resulting pressure drop is an important capital vs. operating cost tradeoff for cost optimization. Therefore, in the final work, a more detailed exchanger model will be used to study the effects of solvent flashing in the exchangers and to more accurately model pressure drop.

The model of the Advanced Flash Stripper consists of two single-stage equilibrium flash blocks representing the steam heater (reboiler) and condenser. The packing is represented with the same rate-based packing mass transfer model used in the absorber. Thermodynamic and mass transfer properties can be adjusted for the stripper separately from the absorber to better model the different operating conditions of the stripper. Validating the stripper portion of the model and making the necessary adjustments is an area for future work.

This constitutes a model of the full capture process with a closed solvent recycle loop which closes the mass and energy balance of the process. The model is equation-oriented, meaning that the complete process is represented by a set of equations which are solved simultaneously. This eliminates the need for an iterative solution method using stream tearing.

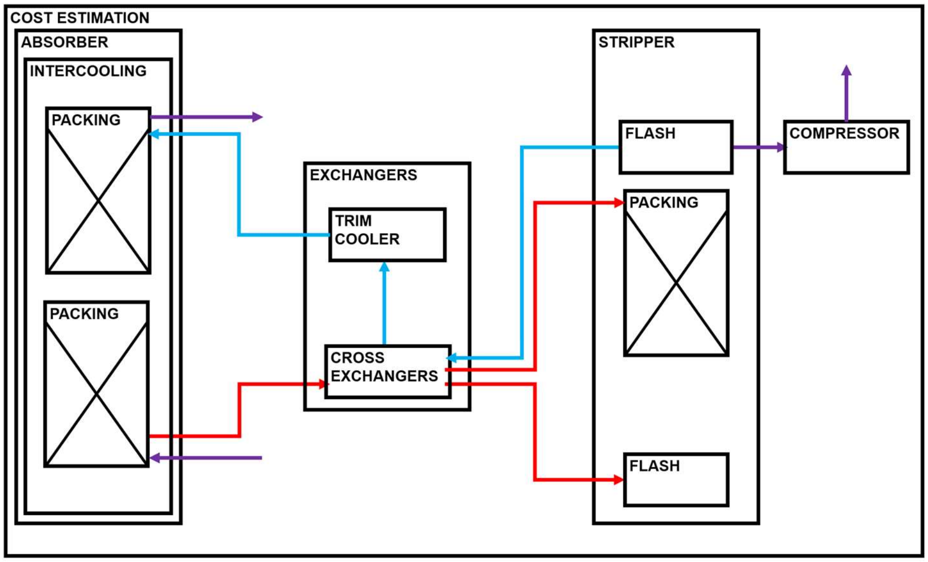

Figure 2: Hierarchy of modules within the full-flowsheet model. Streams within modules omitted for clarity.

Sensitivity analysis

In the present abstract, simplified models are used for the heat exchangers and stripper. Finalizing these models is necessary before equipment cost and energy consumption can be modeled for cost optimization. As a preliminary step to the final optimization task, sensitivity analysis was performed to study the effect on absorber performance of varying key design or operating conditions. The following case represents a design using the same (NGCC) flue gas flow and conditions as the Mustang FEED[5]. One important design decision is the packing height of the absorber. Reducing packing height decreases capital cost of the column but increases operating cost by requiring a higher solvent circulation rate for the same capture rate. Figure 3 shows the effect of varying total packing height on solvent circulation rate and rich loading. The following variables are held constant: solvent concentration (5.0 molal), lean loading (0.2), CO_2 removal (95%), and the location of the pumparound intercooling (equivalent to the ratio of heights of the two packed beds).

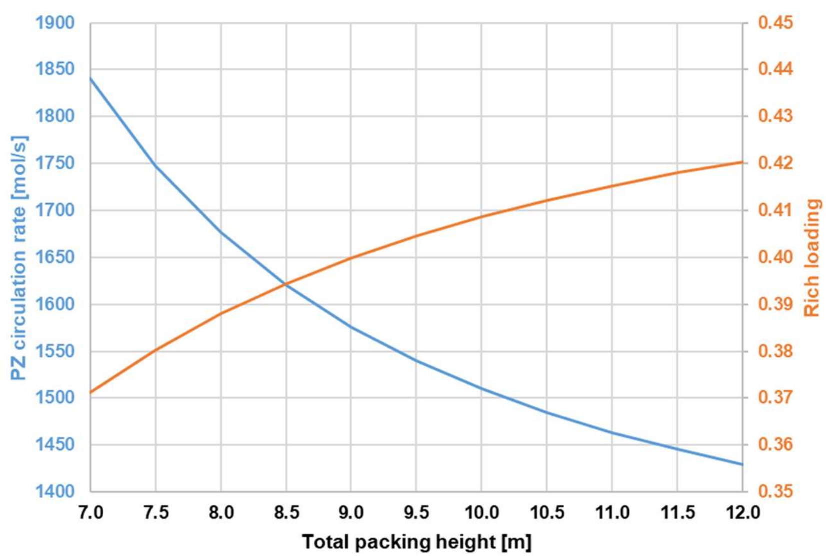

Figure 3: Effect of varying packing height on solvent circulation rate and rich loading at constant capture rate.

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One author of this paper consults for a process supplier on the development of amine scrubbing technology. The terms of this arrangement have been reviewed and approved by the University of Texas at Austin in accordance with its policy on objectivity in research. One author has financial interests in intellectual property owned by the University of Texas that includes ideas reported in this paper.

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