Solid formation in piperazine rate-based simulation

Piperazine is a promising solvent for reducing CO2 emissions. It can be applied for the post-combustion capture process and it has limited degradation and fast kinetics. However, precipitation and slurry formation still represent a challenge for the PZ-CO2-H2O system from an operational point of view but also from a modeling perspective. The present work develops a rate-based model for CO2 absorption and desorption modeling for gas-liquid-solid systems and it is demonstrated for the piperazine CO2 capture process. This model is an extension of the DTU CAPCO2 model to precipitating systems. It uses the extended UNIQUAC thermodynamic model for phase equilibria and thermal properties estimation. The mass and heat transfer phenomena is implemented in a film model approach, based on second order reactions kinetics. The transfer fluxes are calculated using the concentration of the dissolved species since the piperazine is deactivated when present as solid. It is assumed that solid-gas reactions are slow compared to normal liquid side reactions. In the current work, the formation of solids is described in an equilibrium approach, assuming instantaneous formation of hydrates such as PZ·6H2O, PZ·½H2O, and anhydrous PZ. The simulation of a 100t/hr post-combustion capture plant outlines that 5 % solid reduces the CO2 capture rate with 13%. Therefore, it demonstrates that an accurate description of the precipitation phenomenon is essential for realistic and accurate modeling.