Ability of Modern Equation-of-State Models to Correlate and Predict the Properties of Physical Solvents for Acid Gas Removal

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Physical solvents such as dimethyl ethers of polyethylene glycol, N-methyl-2-pyrrolidone, methanol, propylene carbonate, and morpholine derivatives are becoming attractive as gas treating solvents, especially for integrated gasification combined cycle (IGCC) and blast furnace gas (BFG) applications. At high concentrations of acid gases in the feed, physical solvents are favored over chemical solvents due to their non-corrosive nature as well as lower energy costs for solvent regeneration from pressure reduction as opposed to the addition of external heat. The intermolecular interaction of acid gases such as CO_2 with these physical solvents is often characterized by a specific association such as a Lewis acid-base complex with the alcohol or ether sites on the solvent. Modern equation-of-state models such as those based on associated-fluid theory (SAFT) are, in principle, well-suited to describe the phase equilibrium of acid gases with the physical solvents. In this work, we will present the ability of a SAFT-based equation-of-state and a cubic-plus-association (CPA) equation-of-state to correlate the properties of physical solvents, both as pure components and gas-loaded solutions. We will take a close look at the description of gas-liquid equilibrium and the prediction of multicomponent effects of mixed-gas solubilities based on binary data alone. Finally, we will show the potential to develop generalized correlations using these equation-of-state models for the solubility of CO_2 in a series of ethers.