A soft-SAFT Robust Model for the Thermodynamic Characterization of CO_2 Absorption in Aqueous Mixtures of Amines

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Aqueous mixtures of amines are considered to be the gold standard solvents for the removal of CO_2 from the gas streams of many industrial processes such as natural gas production, gas ammonia synthesis and power generation from fossil fuels. The capture/release process involves the cyclic chemical absorption of CO_2 at temperatures ranging from 303 to 323 K, and regeneration of the CO_2-rich solvent at higher temperatures, typically in the range 373-393 K. To make the application of amine-based separation processes at a large scale more effective, given the range of possible amines and formulations, it is necessary to develop an accurate and consistent method for predicting the phase behavior and thermophysical properties of this class of solvents, including the solubility of CO_2 in them. In this communication, a robust theoretical framework based on the soft-SAFT equation of state has been used for modeling the phase equilibria of several aqueous amines, including MEA, AMP, DEA, MDEA and PZ, at conditions of relevance for industrial applications. In the model, the complex hydrogen-bonding behavior between water-amine and amine-amine pairs have been characterized by association parameters transferred from monofunctional molecules, significantly reducing the number of fitted parameters, and the chemisorption of CO_2 described in terms of the formation CO_2-amine aggregates through strong intermolecular association interactions. The capabilities of the EoS have been extended for the computation of viscosities and interfacial properties by coupling with the Free-Volume Theory and Density Gradient Theory, respectively. The model has been found to provide an accurate representation of the effects of association interactions in the systems' non-idealities, with most of the mixture properties being obtained in a fully predictive manner and found to be in good agreement with experimental data of both single and blended amine solutions, being well-suited for the study of other amines.