Analysis of thermodynamic models for amine-based CO_2 absorption process

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A reliable thermodynamic model capable of describing thermodynamic properties for mixtures of amine, water and CO_2 is essentially required to design and simulate the amine-based CO_2 absorption process. In this work, a Kent-Eisenberg and an electrolyte NRTL as representative models are studied to analyze phase behaviors (vapor-liquid equilibria, chemical reaction equilibria) and thermal properties (heat of mixing, heat of absorption, heat capacity) of the systems by comparing the calculation results with literature data. For MEA solutions chosen as the basic system, molecular components are in equilibrium between vapor and liquid phases according to the physical solubility, while the distribution of species in aqueous phase is determined by five chemical equilibrium constants. The Kent-Eisenberg is the simplest model by assuming ideal gas and solution and lumping the non-ideality of the aqueous phase into the chemical equilibrium constants fitted to experimental data. The electrolyte NRTL is relatively rigorous compared to other existing models but it can give more accurate description on concentrations of true species in the aqueous phase improving the performance of a rate-based simulation. Reference state for each component of the system is carefully considered in the electrolyte NRTL.