

Modeling of Enthalpy of Solution of Carbon Dioxide in Aqueous Solution of Amine

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The {CO₂-H₂O-amine} systems are of interest in order to develop carbon dioxide (CO₂) capture processes. Because of environmental impact, particularly for global warming effect, CO₂ emissions have to be limited. One option is to remove CO₂ from post combustion effluent in industries such as cement, metallurgy or power plants. The most common processes are based on cycles of gas absorption in amine solution and regeneration of the solution in a stripper. The economical cost of the second step must be reduced in order to develop the CO₂ treatment in the industry. The regeneration is performed by heating the solution. The required energy for gas desorption is directly related to the enthalpy of solution of CO₂ in the amine solution. Direct measurements of enthalpy of solution are not easy to carry out and experimental data are relatively scarce compared to vapor-liquid equilibrium (VLE) data. The objective of this work is to analyze how enthalpy of solution can be calculated from available VLE data. The mechanism of gas absorption is a combination of chemical reactions and physical absorption that can be described by thermodynamic models⁽¹⁻³⁾. The chemical and physical equilibria are represented using chemical equilibrium constants and Henry's constants obtained from literature. The none-idealities in the liquid and gas phases are taken into account using a *g-f* approach. In a first step, the interaction parameters, used in the model for the calculation of activity coefficients⁴, are adjusted to correlate the VLE data. Then, the enthalpies of solution are derived⁵ from the equilibrium equations using thermodynamic relationship. The calculated values are compared with experimental data⁽⁶⁻⁷⁾. The total enthalpy of solution is divided in several contributions related to amine protonation, CO₂ and water dissociation and gas-liquid equilibria. These enthalpy contributions are obtained, among others, from the temperature derivations of the related equilibrium constants. When different temperature correlations are available in the literature for the same constant, the influence on the calculated enthalpy is analyzed.

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