Mechanism of CO_2 Absorption in Aqueous Solutions Containing Three Alkanolamines: Experimental and Thermodynamic Modeling Approaches

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Alkanolamines are classified into primary, secondary, ternary and steric-hindrance amine according to the number of amine group. The absorption mechanism of CO_2 in an aqueous solution containing three alkanolamines was analyzed experimentally and theoretically. The vapor-liquid equilibrium was evaluated experimentally over a wide temperature range at several blending ratios. The successive substitution method was used to calculate the concentrations of molecules and electrolytes (for cations and anions) in the liquid phase by solving chemical equilibrium equations, mass balance equations and charge balance equation. The Deshmukh-Mather model, which is based on an activity coefficient approach, and fugacity coefficient model were used to evaluate the non-ideality of the liquid and vapor phases, respectively. Thereafter, the effect of the blending ratio was evaluated using the triangular diagrams of the carbamate, bicarbonate and carbonate molar fractions in liquid phase, CO_2 loading ratio, CO_2 cyclic capacity, and heat of CO_2 absorption. Calculations of simulation results were conducted by MATLAB® 2020a version.