Enthalpy of Absorption and Vapor-Liquid Equilibrium of the CO_2-MDEA-H_2O System

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Acid gases (mainly CO_2 and H_2S) are usually removed from gaseous streams by countercurrent contact with an aqueous amine solution. This is a consolidated industrial technology and is preferred to physical absorption because of the presence of the amine in the liquid phase, which undergoes to chemical reactions and so enhances the mass transfer. Due to the exothermicity of reactions, a temperature increase occurs in the absorber, affecting the equilibrium and the amount of absorbed acid gas, while in the regenerator the energy requirement at the reboiler strongly depends on the heat of desorption. A correct information on the enthalpy, then, is fundamental to design the acid gas removal section of an industrial plant, mainly in an energy saving perspective. The aim of the work is the analysis of the thermodynamics of the system composed of CO_2, water and methyldiethanolamine (MDEA), a tertiary amine widely used also if a separate removal of H_2S and of CO_2 is desired. The study is focused on the computation of the heat of absorption, which, in the open literature, is a field less investigated than the one related to VLE calculations. It is related to the description of the Vapor-Liquid Equilibrium, performed with the Electrolyte-NRTL model, and thus of the adopted VLE parameters. New parameters have been obtained and checked against experimental data of VLE and of heat of absorption. They can be implemented in the commercial software ASPEN Plus® and employed for simulations of the amine scrubbing scheme.