Extended UNIQUAC model for thermodynamic modeling of CO2 absorption in aqueous alkanolamine solutions

The extended UNIQUAC model [K. Thomsen, R Rasmussen, Chem. Eng. Sci. 54 (1999) 1787-1802] was applied to the thermodynamic representation of carbon dioxide absorption in aqueous monoethanolamine (MEA), methyldiethanolamine (MDEA) and varied strength mixtures of the two alkanolamines (MEA-MDEA). For these systems, altogether 13 interaction model parameters are adjusted. Out of these parameters, 11 are temperature dependent. All the essential parameters of the model are simultaneously regressed to a collective set of data on the single MEA and MDEA systems. Different types of data are used for modeling and they cover a very wide range of conditions. Vapor-liquid equilibrium (VLE) data for the aqueous alkanolamine systems containing CO2 in the pressure range of 3-13,000 kPa and temperatures of 25-200 C are used. The model is also regressed with the VLE and freezing point depression data of the binary aqueous alkanolamine systems (MEA-water and MDEA-water). The two just mentioned types of data cover the full concentration range of alkanolamines from extremely dilute to almost pure. The experimental freezing point depression data down to the temperature of -20 degrees C are used. Experimental excess enthalpy (H-E) data of the binary MEA-water and MDEA-water systems at 25, 40, 65 and 69 degrees C are used as well. In order to enhance the calculation of the infinite dilution activity coefficients of MEA and MDEA, the pure alkanolamines vapor pressure data in a relevant temperature range (up to almost 230 degrees C) are included in the parameter estimation process. The previously unavailable standard state properties of the alkanolamine ions appearing in this work, i.e. MEA protonate, MEA carbamate and MDEA protonate are determined. The concentration of the species in both MEA and MDEA solutions containing CO2 are predicted by the model and in the case of MEA compared to NMR spectroscopic data.

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