

Activity Coefficients of the Constituents of Model Wastes of Organic Solvents and Electrolytes. Part II: Phase Equilibria Predictions

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Phase equilibrium of solvent mixtures containing electrolytes is poorly understood, in spite of the need for such data in the design of processes such as crystallization and adsorption. Even a small amount of nonvolatile salt added to a binary solvent mixture can greatly alter the volatility of the solvent components in the mixture [1]. Activity coefficient data at infinite dilution γ^∞ for water-organic-solvent mixtures with varying salt concentrations have been fitted to a modified form of the nonrandom two-liquid (NRTL) equation proposed by Chen et al. [2] that explicitly includes electrolyte (salt) constituents when present. Aqueous binary systems of isopropanol, acetone, and methyl ethyl ketone are examined isothermally at 25 °C using a static equilibrium cell apparatus in the dilute region of each constituent (less than 1.0 mole % solute) to determine γ^∞ at sodium nitrate salt levels of 0.1 - 4.0 molal.

The optimized values of nine binary interaction parameters (BIPs) for these aqueous binary systems are used to estimate the activity coefficients, vapor concentrations and system pressures in highly nonideal mixtures of electrolytes and nonelectrolytes. The predictions are validated with experimental vapor-liquid equilibrium data [3]. In this work, the authors also propose an approach for rigorously optimizing values of BIPs that can accurately predict the LLE as well as the VLE behavior of ternary electrolyte systems.

KEY WORDS: Vapor-Liquid Equilibrium (VLE), Liquid-Liquid Equilibrium (LLE), Mixed Solvents Containing Electrolyte, Activity Coefficient, Hydrophilic Chemicals