

Modeling of phase equilibria with imidazolium based ionic liquids and CO<sub>2</sub> by group contribution non-random lattice fluid equation of state

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Ionic liquids are receiving growing attentions as alternative solvents. Appreciations of thermodynamic properties and phase equilibria involving ionic liquids are needed for applications of operations and designs for chemical processes. In the recent years, experimental phase equilibria data containing ionic liquids have been reported. Sometimes accuracies in equilibrium data were questioned due to their impurities and degradation. These equilibrium data have been mainly modeled by excess Gibbs functions. Equation of state approaches are more convenient to model the phase equilibria of ionic liquids with supercritical gases such as carbon dioxide. In the present study the phase equilibria of imidazolium based ionic liquids and carbon dioxide were modeled by the group contribution non-random lattice fluid equation of state. Group segment numbers and interaction energy parameters between groups were fitted to experimental solubility data and densities of ionic liquids. The agreements between experimental data and calculated solubilities were found generally good. In addition, discrepancies between experimental data in literature were discussed.