

Modeling of the Carbon Dioxide Solubility in Imidazolium-Based Ionic Liquids with the tPC-PSAFT Equation of State

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An equation of state (EoS) is developed to predict accurately the phase behavior of ionic liquid + CO₂ systems based on the truncated Perturbed Chain Polar Statistical Associating Fluid Theory (tPC-PSAFT) EoS. This EoS accounts explicitly for the dipolar interactions between ionic liquid molecules, the quadrupolar interactions between CO₂ molecules and the Lewis acid-base cross-association between the ionic liquid and the CO₂ molecules. Physically meaningful model pure component parameters for ionic liquids are estimated based on literature data. All experimental vapor-liquid equilibrium data are correlated with a single linearly temperature-dependent binary interaction parameter. The ability of the model to describe accurately carbon dioxide solubility in various 1-alkyl-3-methylimidazolium-based ionic liquids with different alkyl chain length and different anion at pressures from 0 MPa to 100 MPa and carbon dioxide fractions from 0 mole % to 75 mole % is demonstrated. In all cases, good agreement with experimental data is obtained.