Prediction of Ammonia Solubility in Ionic Liquids Using UNIFAC Model

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Abstract

Ionic liquid is a new type of green solvent, because of the nonvolatility, good dissolution properties, and high chemical stability. It is expected to replace the current extensive use of volatile solvents, to design environmental friendly new chemical process. However each cations and anions different from each other, combination into a huge number of ionic liquids, if its physical and chemical properties determined through the experiment, the cost is high. So it is highly needed to develop an effective and reliable method to predict the thermodynamic properties of the systems containing ionic liquid. Ammonia (NH₃) solubility studies about the design and production of natural gas plays an important role. In this paper the solubility of NH₃ in different ionic liquids are studied, and compared with the results predicted by UNIFAC model.

The accurate calculation of the NH₃ solubility in ILs is important in natural gas purification. UNIFAC model is selected to predict the solubility of NH₃, which can decrease a plenty of experimental work in the laboratory. The new group NH₃ is defined by regression of the experimental data collected from the literatures published to obtain the group-group interaction parameters between the components of NH₃ and ionic liquids. The consistency test is carried out to examine the accuracy of prediction results. The solubility predicted by UNIFAC model is verified a perfect agreement with the experimental data provided in the literature at temperature range from 282.2 K to 355.8 K and pressure up to 25 bar, with an average relative deviation (ARD) less than 10 %. The results demonstrate that for system studied in this work, UNIFAC model can realize the solubility prediction successful. This predictive model is useful for predicting the NH₃ solubility in imidazolium-based ionic liquids and providing the phase equilibrium data for the application of liquid natural gas and the relevant mass transfer separation in chemical engineering.