

Prediction of Ionic Liquid Densities Using a Corresponding State Correlation

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Abstract : Ionic liquids (ILs) exhibit particular properties exemplified by extremely low vapor pressure and high thermal stability. The properties of ILs can be tailored by proper selection of cations and anions. As such, ILs are appealing as potential solvents to substitute traditional solvents with high vapor pressure. One of the IL properties required in chemical and process design is density. In developing corresponding state liquid density correlations, scaling hypothesis is often used. The hypothesis expresses the temperature dependence of saturated liquid densities near the vapor-liquid critical point as a function of reduced temperature. Extending the temperature dependence, several successful correlations were developed to accurately correlate the densities of normal liquids from the triple point to a critical point. Applying mixing rules, the liquid density correlations are extended to liquid mixtures as well. ILs are not molecular liquids, and they are not classified among normal liquids either. Also, ILs are often used where the condition is far from equilibrium. Nevertheless, in calculating the properties of ILs, the use of corresponding state correlations would be useful if no experimental data were available. With well-known generalized saturated liquid density correlations, the accuracy in predicting the density of ILs is not that good. An average error of 4-5% should be expected. In this work, a data bank was compiled. A simplified and concise corresponding state saturated liquid density correlation is proposed by phenomena-logically modifying reduced temperature using the temperature-dependence for an interacting parameter of the Soave-Redlich-Kwong equation of state. This modification improves the temperature dependence of the developed correlation. Parametrization was next performed to optimize the three global parameters of the correlation. The correlation was then applied to the ILs in our data bank with satisfactory predictions. The correlation of IL density applied at 0.1 MPa and was tested with an average uncertainty of around 2%. No adjustable parameter was used. The critical temperature, critical volume, and acentric factor were all required. Methods to extend the predictions to higher pressures (200 MPa) were also devised. Compared to other methods, this correlation was found more accurate. This work also presents the chronological order of developing such correlations dealing with ILs. The pros and cons are also expressed.

Keywords : correlation, corresponding state principle, ionic liquid, density

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