Modeling Tetra-n-butyl ammonium halides aqueous solutions with the electrolyte cubic plus association equation of state - DTU Orbit (05/10/2019)

This work presents the thermodynamic modeling of the fluid phases of Tetra-n-butyl ammonium halides aqueous solutions with the electrolyte Cubic-Plus-Association (e-CPA) Equation of State (EOS). The adjustable model parameters are obtained by fitting the experimental data of mean ionic activity coefficients and osmotic coefficients. Several other thermodynamic properties of the aqueous solutions, such as relative static permittivity, liquid density and saturation pressure, are subsequently predicted by the e-CPA EOS. The results of Tetra-n-butyl ammonium bromide aqueous solution show that the model can satisfactorily correlate the mean ionic activity coefficients and osmotic coefficients with the percentage average absolute deviations being 7.2% and 5.9%. The model overpredicts the liquid density with a deviation of 9.2%, while it can correlate the liquid density within 0.2% with a volume translation parameter. In order to have a more complete picture of the capabilities and limitations of the model, the consistencies of experimental data, parameter estimation approaches and the ion sizes are extensively analyzed and discussed.

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