A Thermodynamic Modelling Study of Aqueous Tetra-n-butyl Ammonium Halide Solutions

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This work presents a novel model for aqueous electrolyte solutions that extends the Cubic Plus Association Equation of State by combining the Debye–Hückel theory for electrostatic interactions. This model is applied to perform a fluid phase modelling study of aqueous tetra-n-butyl ammonium halide solutions. The interaction parameters between cations/anions and water are evaluated by regression of the experimental mean ionic activity coefficients (MIAC) of the electrolyte. The results show that this novel model correlates reasonably well with the experimental MIAC (for example, the relative average deviations are 6.3% for the MIAC of tetra-n-butyl-ammonium bromide). The interaction parameters between cations/anions and gas are evaluated by regression of the experimental gas solubilities. The results show that this novel electrolyte model correlates reasonably well with gas solubility (for example, the relative average deviations are 2.9% for the nitrogen solubility in aqueous tetra-n-butyl-ammonium bromide solutions). For a more complete evaluation of the model, the electrostatic terms, parameter estimation approaches, and salting effects on gas solubility are analysed and discussed in detail.

Keywords: Aqueous Tetra-n-butyl Ammonium Halide Solutions; Electrolyte Equation of State; Debye–Hückel Theory; Hydrophobic Effect

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