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Modeling of Dielectric Properties of Aqueous Salt Solutions with an Equation of State - DTU Orbit (09/11/2017)

Modeling of Dielectric Properties of Aqueous Salt Solutions with an Equation of State

The static permittivity is the most important physical property for thermodynamic models that account for the electrostatic interactions between ions. The measured static permittivity in mixtures containing electrolytes is reduced due to kinetic depolarization and reorientation of the dipoles in the electrical field surrounding ions. Kinetic depolarization may explain 25–75% of the observed decrease in the permittivity of solutions containing salts, but since this is a dynamic property, this effect should not be included in the thermodynamic modeling of electrolytes. Kinetic depolarization has, however, been ignored in relation to thermodynamic modeling, and authors have either neglected the effect of salts on permittivity or used empirical correlations fitted to the measured static permittivity, leading to an overestimation of the reduction in the thermodynamic static permittivity. We present a new methodology for obtaining the static permittivity over wide ranges of temperatures, pressures, and compositions for use within an equation of state for mixed solvents containing salts. The static permittivity is calculated from a new extension of the framework developed by Onsager, Kirkwood, and Fröhlich to associating mixtures. Wertheim's association model as formulated in the statistical associating fluid theory is used to account for hydrogen-bonding molecules and ion–solvent association. Finally, we compare the Debye–Hückel Helmholtz energy obtained using an empirical model with the new physical model and show that the empirical models may introduce unphysical behavior in the equation of state.

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