Quantifying the Effect of Polar Interactions on the Thermophysical Properties of Selected Model and Experimental Systems

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It is well known that polar interactions play a key role on the thermophysical properties of pure fluids and their mixtures, leading to great deviations with respect to their ideal behavior. However, in experimental systems it is sometimes difficult to isolate the effect of the polar interactions from other non-ideal interactions. Conversely, molecular-based theories and molecular simulations can help in this regard, as the different contributions to the total intermolecular forces can be isolated and quantified. In this work, we present the polar soft-SAFT Equation of State where intermolecular polar interactions (dipolar and quadrupolar) are explicitly considered. After a brief introduction of the theory, we will present results concerning its validation against molecular simulation data with the same underlying models, in a purely predictive manner, for a wide range of pure polar model systems such as Stockmayer fluids, LJ dimers with dipole and quadrupolar LJ fluids, for a range of thermophysical properties such as liquid density, vapor pressure, surface tension and heat capacities. Additionally, the phase equilibria and surface tension of a wide range of binary mixtures of model polar fluids are also validated against molecular simulations. Once the accuracy of the theory is proven, it is then applied in a predictive and systematic manner to isolate the effect of polar interactions (dipolar and quadrupolar) on the phase equilibria, surface tension, and density profiles of binary mixtures of nonpolar, dipolar, and quadrupolar model fluids. Lastly, the equation was applied to calculate a range of thermophysical properties of pure polar fluids and their mixtures with other substances, including VLE, surface tension and second-order derivative properties, finding good agreement with experimental data.

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