

Molecular Modeling of Fluids: Simple Models of Polar and Associating Fluids and Their Applications

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Simple models result usually from speculative or intuitive speculations. We have recently developed a theoretical method enabling one to construct simple models (called primitive models) as direct descendants of realistic intermolecular interaction models of complex (polar and associating) fluids. The primitive models (i) reproduce faithfully (semi-quantitatively) the structure of their realistic parent models, (ii) are amenable to a theoretical treatment using the thermodynamic perturbation theory, and (iii) capture also a good deal of their thermodynamic properties (typically 90% or more). Besides their direct use as a reference in perturbation theories, the primary use of primitive models is to study and elucidate complex processes at molecular level in the same way the model of hard spheres does for simple fluids.

Application of the primitive models is exemplified (i) by studying the structure and thermophysical properties of various aqueous systems, and (ii) by deriving a perturbed equation of state of water and alcohols that reproduce real experimental data including their anomalies.