A Molecular Based Approach to Modeling Complex Fluids

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The development of a predictive molecular-based description of the thermodynamic properties of complex fluids is central to modeling systems in both traditional and emerging industries. To address this need, we have been developing the variable-range version (VR) of the statistical associating fluid theory (SAFT), known as SAFT-VR, into a tool that can describe the thermodynamic properties and phase equilibria of a wide range of complex molecular systems (ranging from simple fluids to hydrocarbons, alcohols, polymers, and water, as well as mixtures of these systems) at state conditions ranging from ambient to supercritical, including the critical point. We develop these additional capabilities for SAFT-VR by incorporating advances in molecular theory (e.g., crossover theory for the critical point and integral equation theory for dipolar and electrostatic interactions). In order to test the accuracy of the resulting SAFT-VR thermodynamic models, at each step we use molecular simulation to test their accuracy before then applying the resulting SAFT-VR theory to real systems. This ability to test SAFT-VR against molecular simulation of the same molecular model is the key to its success, and distinguishes SAFT based approaches from other classical engineering tools to modeling thermodynamic properties. We describe several examples of the process of incorporating advances into SAFT-VR, validating them by molecular simulation, and then applying them to real systems.