

238d Phase Behavior of Dipolar Fluids from the Saft-Vr Equation of State

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In order to develop a truly predictive approach for the thermophysical properties and phase behavior of real fluids we need to incorporate the molecular interactions explicitly into the equation of state. As a move towards this goal we have extend the SAFT-VR approach to explicitly account for dipolar interactions. Predictions for the thermodynamic properties and phase behavior of dipolar square-well monomer and chain fluids in which one or more segments is dipolar are considered. The mean spherical approximation is used to account for the long-range Coulombic dipolar - dipolar interactions.

Isothermal-isobaric and Gibbs ensemble Monte Carlo simulations have been performed to test the theoretical approach on model fluids before application to real systems. The computer simulations show that the equation of state provides a good description of the phase behavior of dipolar monomer and chain molecules at relatively low dipole moment and for fluids with a large overall dipole moment. In order to improve predictions for higher dipole moments higher order versions of the MSA are used. Preliminary results will be presented for the application to real fluids.

Keywords: SAFT EOS, MSA, dipolar interaction, NPT MC and GEMC simulations, phase diagram