Molecular Modeling of Fluids Near to and Far from the Critical Region: Application of SAFT-VRX

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Today there exists a wide range of classical equations of state (EOSs), which, with parameters fitted to experimental data, can accurately predict the phase behavior of fluids and their mixtures in the region away from the critical point. Perhaps the most versatile of these is the molecular-based SAFT-VR EOS, which has been shown to be capable of predicting fluid phase equilibria in a wide variety of pure and mixed fluid systems, including non-polar (*e.g.*, noble gases and methane), polar (*e.g.*, alcohols), hydrogen-bonding (*e.g.*, water and HF) and chain fluids (*e.g.*, alkanes and polymers). As such, it is perhaps the most versatile fundamentally based engineering EOS in use today. However, in common with all analytic EOSs, SAFT-VR exhibits classical behavior in the critical region rather than the non-analytical, singular behavior seen in real fluids. Recently, so-called crossover equations of state have been developed to solve this shortcoming by incorporating the scaling laws valid asymptotically close to the critical point while reducing to the original classical equation of state far from the critical point. In this work, we have combined the SAFT-VR EOS with a recently proposed crossover technique developed by Kiselev *et al.* to obtain the SAFT-VRX EOS. The SAFT-VRX approach combines the accurate low-temperature behavior of SAFT-VR with an accurate representation of the critical region. Results will be presented for both non-associating and associating fluids, such as hydrocarbons, water and alcohols, and compared with both experimental data and the original SAFT-VR approach.