Evaluation of equations of state for simultaneous representation of phase equilibrium and critical phenomena

Precise description of the critical points with association equations of state requires rescaling of the parameters to match experimental critical temperature and pressure of pure components. In this work we developed a method to include critical data restrictions in the parametrization procedure of the Cubic-Plus-Association (CPA) equation of state (EoS). We obtained new parameters for methanol and alkanes from n-hexane to n-decane. The comparison with the original parameters showed that this procedure is important for associating compounds, since for inert species the equation reduces to the Soave-Redlich-Kwong (SRK) EoS. The application of the rescaled parameters improved the critical point representation of pure fluids at the expense of the saturated liquid phase volume description. In the case of binary mixtures containing methanol and n-alkanes, the association model with the new parameters satisfactorily predicted the experimental critical data, indicating the importance of the rescaling parametrization procedure in the computation of the critical pressure and temperature for systems with associating species. Both sets of CPA parameters gave similar deviations in the bubble point pressure and vapor composition for the vapor-liquid equilibrium calculations. However, the rescaled parameters gave rise to larger deviations in the composition of the polar rich phase in the liquid-liquid equilibrium.

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