87a Tracing the Critical Locus for Binary Fluid Mixtures Using Molecular Simulations

Philip J. Lenart and Athanassios Z. Panagiotopoulos

Phase behavior at high temperatures and pressures have numerous applications,particularly in separation processes. Numerous studies have employed the use of equations of state to determine the critical locus for a binary mixture, but little work has been done using molecular simulation. We determine the critical locus for a variety of binary mixtures including non-polar, polar, and ionic species using grand canonical Monte Carlo simulations with histogram reweighting. The critical point is determined using the finite-size scaling approach of Bruce and Wilding [1]. Different classes of the critical locus in binary mixtures, such as Class I and Class IIIb, are seen for systems including methane-ethane, methane-water, and water-NaCl. The choices for the intermolecular potentials and the combining rule between species have a significant impact on the critical locus. Finally, the effect of including polarization in the methane-water mixture on the critical locus is presented.

1. A.D. Bruce and N.B. Wilding, Phys. Rev. Lett. 68, 193 (1992).