148h First-Order Mean Spherical Approximation and Its Application to the Critical Region

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The first-order mean-sphere approximation (FMSA) is an analytical theory to study homogeneous and inhomogeneous fluids through two fundamental pieces of information – radial distribution function (RDF) and direct correlation function (DCF). With RDF being essential to develop an accurate classic equation of state, DCF is vital to investigate inhomogeneous behavior such as interfacial phenomena, molecules nearby walls and around colloidal particles. The decisive role of DCF can be further viewed in studying complex non-classic behavior inside the critical region. Very recently, Mi et al. (AIChE J., in press) integrate renormalization group (RG) theory with DCF to describe long-range density fluctuations. The new RG theory is applied to correcting mixture phase envelops, as well as corresponding phase diagrams of pure compounds for the critical region. The calculated results are in very good agreement with from experiment and computer simulation both inside and outside the critical region. The new method is highly predictive since no adjustable parameters and no mixing rules are needed for both model and real fluid mixtures. Therefore, FMSA represents a unified framework to handle these classic and non-classic phenomena, as well as those traditional inhomogeneous behaviors.