Modifying Veytsman for long-range fluctuation in critical region

이주호, 신문삼, 김화용* 서울대학교 응용화학생물공학부 (hwayongk@snu.ac.kr*)

Lattice fluid models are capable of describing complex systems such as polymers and hydrocarbon compounds1. But the models fail to correctly explain the equilibrium properties at critical region because the short-range interaction is considered and long range fluctuation dominant at such condition ignored. The long range fluctuation has been successfully described by crossover models or renormalization group theory. They, however, are only developed on the basis of cubic or hard sphere chain equation of states. To apply lattice fluid model into critical region, it is required to include long range fluctuation. In this work, we modified athermal chain contribution (repulsive part) with the molecular simulation data of tangent hard sphere chain and Veytsman statistics to account for density fluctuation at critical region by introducing new probability factor. The development model showed a good agreement with two coexistence and single phase data of methane.