New Optimized Potentials for Phase Equilibria with Enhanced Predictability

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United atom force field such as TraPPE (transferable potentials for phase equilibria), OPLS (optimized potentials for liquid simulation) and NERD has been providing the substantial template for the fast and accurate molecular simulation of phase equilibria. In particular, TraPPE is known for its highly accurate predictability for hydrocarbon by which it has remained undeniably the best force fields for phase equilibria simulation. However, it is parameterized to estimate the liquid density and critical temperature of the pure hydrocarbon fluid. So, this potential model fails to predict the vapor phase density and vapor pressure of hydrocarbon. In addition, it tends to overestimate liquid density for hydrocarbon longer than 8~12 chain length. To overcome this flaw, the intra- and inter-molecular interaction parameters were determined with consideration of both the liquid density and vapor pressure. The phase equilibria simulation results with the newly optimized parameters set show excellent agreements with the experimental vapor-liquid coexistence data. Especially, our results were comparable or better than those by TraPPE in terms of the predictability.