Understanding Phase Behaviors of Multicomponent Polymer Mixtures and Hydrocarbon Mixtures Based on a Molecular Thermodynamic Framework

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A new molecular thermodynamic model based on a closed-packed lattice model is developed for multicomponent systems. Based on Monte-Carlo (MC) simulation results, we introduce new universal functions to consider the chain length dependence of chain molecules, and are able to obtain more accurate critical volume fraction results in liquid-liquid equilibrium (LLE) calculations. To minimize the number of adjustable model parameters, chain length parameters are calculated in a conventional way using molecular weight and specific volume. Our proposed model successfully describes binary LLE for polymer-solvent systems, and the model parameters obtained from these binary systems are directly used to predict corresponding LLE ternary systems. Furthermore, we extend this model to describe PVT properties, such as vapor-liquid equilibrium (VLE). To consider the effect of pressure on the phase behavior, the volume change effect is taken into account by introducing holes into the incompressible lattice model with two mixing steps. The corresponding lattice fluid equation of state (LF-EoS) is applied to predict the thermodynamic properties of pure and binary hydrocarbons systems as well as pure polymer solutions.