

Thermodynamic Modeling for Ternary Liquid-Liquid Equilibrium (LLE) of Simple Liquids and Polymer Mixtures Based on Incompressible Lattice

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A molecular thermodynamic model for multi-component systems based on a closed-packed lattice model is presented based on two contributions; entropy and energy contribution. The calculated liquid-liquid equilibrium (LLE) of ternary chainlike mixtures agreed with Monte Carlo (MC) simulation results. The proposed model can satisfactorily correlate Types 0, 1, 2 and 3 phase separations of the Treybal classification. The model parameters obtained from the binary systems were used to directly predict real ternary systems and the calculated results correlated well experimental data using few adjustable parameters. Specific interactions in associated binary systems were considered using a secondary lattice.