

Simulation of Liquid-Liquid Interfaces

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We perform molecular dynamics simulations to obtain the solubility of n-heptane (C7) and n-decane (C10) in N-methyl-pyrrolidone (NMP) as a function of temperature. Simulations at constant pressure for the liquid phases of NMP and binary mixtures containing C7 and NMP are used to validate the potential parameters of NMP. The difference with experimental densities is less than 5%. The liquid-liquid phase equilibrium of C7-NMP and C10-NMP are analyzed at different temperatures. The composition of each component in every liquid phase is obtained via the density profile. The solubility of C7 and C10 in NMP is greater than the solubility of NMP in the phase rich in hydrocarbon. This finding is in agreement with experimental data. The same procedure is used to obtain the solubility of benzene in ternary mixtures containing C7 and NMP. The surface tension of these interfaces will be discussed.