Closed-loop liquid-liquid immiscibility in mixtures of particles with spherically symmetric interaction

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The investigation of the phase behavior of symmetric binary mixture of Yukawa hard spheres equal size with additional associative spherically symmetric interaction between particles of different species was made. Interactions between the particles of one sort is the same $(U_{11}^{(YU)}(r) = U_{22}^{(YU)}(r))$, and the intensity of attraction between particles of different sorts is regulated by the parameter α , $(0 < \alpha < 1, U_{12}^{(YU)}(r) = \alpha U_{11}^{(YU)}(r))$. The investigation was made in the framework of the high temperature approximation (HTA) [1] and the thermodynamic perturbation theory (TPT) [2],[3]. To calculate radial distribution function we use Grundke-Henderson parametrization for hard sphere mixtures [4] and use direct correlation function obtained from the first-order mean spherical approximation (FMSA) for Yukawa fluids [5]. Calculations of the phase diagrams based on the solution of the equations that follow from the conditions of phase equilibrium, i.e. equal chemical potentials and pressures in coexisting phases. The phase diagrams for different interaction distances less than its value at contact was obtained.

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