

Liquid-gas phase behavior of polydisperse dipolar hard-sphere fluid

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Liquid-gas phase diagram for the dipolar hard-sphere fluid was calculated theoretically more than thirty five years ago by Rushbrooke et al. [1]. According to these calculations the critical point is located at reduced temperature $T_c^* = 0.279$ and reduced density $\rho_c^* = 0.159$. Systematic computer simulation search for the liquid-gas phase coexistence was initiated only twenty years later [2,3]. These investigations were carried out at temperatures well beyond predicted theoretically, however no evidence for the phase transition was found. Shortly after there appeared a number of the theoretical papers, in which the arguments were given as to why the existence of the liquid-gas phase transition has to be ruled out. It was suggested that due to the highly anisotropic character of the dipole-dipole interaction the formation of the chains in the 'nose-to-tail' arrangement suppresses the liquid-gas phase transition. However, recent computer simulation [4], carried out for the temperatures lower than those studied earlier, presented the evidence for the phase transition with the critical point located at $T^* \approx 0.15 - 0.16$ and $\rho^* \approx 0.1$.

We present and discuss the liquid-gas phase diagrams of the monodisperse and polydisperse versions of the dipolar hard-sphere fluid, calculated using thermodynamic perturbation theory for associative fluids with center-center type of interaction [5,6].

1. Rushbrooke G.S., Stell G., Hoye J.S., Mol.Phys. **26**, 1199 (1973).
2. Caillol J.-M., J.Chem.Phys. **98**, 9835 (1993).
3. van Leeuwen M.E., Smit B., Phys.Rev.Lett. **71**, 3991 (1993).
4. Camp P.J., Shelley J.C., Patey G.N., Phys.Rev.Lett. **84**, 115 (2000).
5. Y.V.Kalyuzhnyi, G.Stell. Mol.Phys. **78**, 1247 (1993).
6. Y.V.Kalyuzhnyi, I.A.Protsykevych, P.T.Cummings, EPL **80**, 56002 (2007).