Vapor-Liquid Phase Coexistence Properties for the Triangular Well Fluid of Variable Width

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Equations of state (EoS) based on a two parameters model fall in a description of a corresponding state theory (CS) [1,2], which is not suitable to describe the properties of real fluids. To obtain a non-conformal behavior [1] that breaks down the CS for real fluids, it is necessary to use a three parameter potential. In this work, a fluid with molecules that interact with a triangular well potential of variable width was studied.

The non-conformal behavior of this fluid can be observed by the vapor-liquid equilibrium curve obtained for different values of the well width. No information for the phase equilibrium data of the fluid has been previously reported in the literature.

In this work, the vapor-liquid equilibrium for triangular well fluid was studied by a proposed equation of state based on the perturbation theory. The obtained curves were compared with new molecular simulation data obtained here for this fluid at different well widths. New data for this fluid in the one phase region is also presented.

The proposed EoS describes an equilibrium curve and critical compressibility factor function of the well width. These results are in agreement with the results obtained from molecular simulation.

The phase equilibrium data for a well width of 2 times the sphere diameter are close to those reported for the Lennard-Jones fluid. The proposed model over predicts the critical temperature of the triangular well fluid.

[1] A. Gil-Villegas, F. del Río, and A.L. Benavides, Fluid Phase Equilbria. **119**, 97 (1996).
[2] M. Cismondi, and J. Mollerup, Fluid Phase Equilibria **232**, 74 (2005).