

Liquid-vapor equilibrium and critical temperature of parabolic-well fluids of variable width by Gibbs ensemble Monte Carlo simulation

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Systems of particles interacting via the van Hove potentials have been extensively studied by statistical mechanical methods[1]. Such interest is invariably due to the fact that these potentials are the simplest models which include the presence of attractive and repulsive forces. Nevertheless, the thermodynamic properties of fluids whose molecules interact via van Hove potentials can still offer some interesting results. In a recent paper[2], we addressed such properties for the case of parabolic-well molecular fluids. In this instance, the intermolecular potential between a pair of particles separated by a distance r is given by

$$u(x) = \begin{cases} \infty, & 0 \leq x \leq 1, \\ \epsilon \left[\left(\frac{x-1}{\lambda-1} \right)^2 - 1 \right], & 1 < x \leq \lambda, \\ 0, & x > \lambda, \end{cases} \quad (1)$$

where $x = r/\sigma$ is the reduced distance, σ is the diameter of the hard core, $\epsilon > 0$ is the well depth and $\lambda > 1$ is the potential range, and we derived an approximate equation of state for these fluids using a second-order thermodynamic perturbation theory. The outcome of this approximation for different values of the parameters involved in the potential was tested against simulation results for various isotherms. Here we extend our previous development by further analyzing the liquid-vapor equilibrium and critical temperature of these parabolic-well fluids. By means of Monte Carlo simulation, and using a modification of the

software DL_Monte from the Collaborative Computational Project CCP5 [3, 4], Gibbs ensemble simulations have been performed for three such parabolic-well fluids in which the ranges are $\lambda = 5/4, 3/2$ and $7/4$, respectively. An advantage of the Gibbs ensemble Monte Carlo technique over other computer simulation methods is that a closer proximity to the critical point can be achieved. Finally, We compare and discuss the results with the cases of triangle-well and square-well fluids, as well as our previous estimates of the critical temperature according to the Vliegthart and Lekkerkerker criterion[5, 2].

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