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Wall free energy based polynomial boundary conditions for non-ideal gases lattice boltzmann simulation LIN LIU, City College and Graduate Center of City University of New York, TAEHUN LEE, City College of City University of New York — Intermolecular forces between solid and liquid can be represented by the inclusion of the wall free energy in the expression of the total free energy for the bulk phases. We derived and investigated three types of polynomial (linear, quadratic, and cubic) wall free energy boundary conditions for the non-ideal gas lattice Boltzmann equation (LBE) method. Both static and dynamic drops on solid surfaces are examined. All the proposed boundary conditions are able to predict the equilibrium states very well in the moderate contact angle range by incorporating appropriate potential form of the intermolecular forces and the bounce-back rule that guarantees mass conservation for both static and dynamic cases. Simulations with different boundary conditions are carried out and the results are compared concerning the accuracy as well as the applicability of different boundary conditions. Numerical results show that the cubic boundary condition has the fastest spreading rate among the three types of the boundary conditions, while, due to the neglect of vapor-solid intermolecular forces and the highly elevated liquid density at the hydrophillic surface, the quadratic boundary condition demonstrates the slowest spreading rate.

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