Lattice Boltzmann simulations of the contact angle in a liquid-gas system

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1. Introduction

Recently, the lattice Boltzmann method (LBM) has gained much attention for its ability to simulate fluid flows, and for its potential advantages over a conventional CFD method. The key advantages of LBM are, (1) suitability for parallel computations, (2) absence of the need to solve the time-consuming Poisson equation for a pressure, and (3) an ease with multiphase flows, complex geometries and interfacial dynamics may be treated[1].

The shape of a moving droplet is difficult to investigate analytically because the classical continuum hydrodynamic equations of motion with the usual no-slip condition at the surface predict a singularity in the stress at the contact line[2]. Briant et al. have proposed a wetting boundary condition by using the wetting potential[3].

In this study, we introduce the wetting boundary condition into the LBM proposed by Zheng et al.[4]. The static contact angle of a droplet onto a wall in order to validate the method is calculated. By adopting a finite difference gradient operator of a sufficient isotropy, the spurious currents can be made small in the wall surface. The main objective of the present work is to establish the lattice Boltzmann method as a viable tool for the simulation of multiphase or multi-component flows.

2. Methods and Results

2.1 Methodology

Here, we consider a flow with two phases which have different densities. The low density and high density are noted as ρ_L and ρ_H respectively. The flow can be described by the Navier-Stokes equations and an interface evolution equation as [4]

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \vec{u}) = \theta_M \nabla^2 \mu_\phi \qquad (1)$$

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \vec{u}) = 0 \qquad (2)$$

$$\frac{\partial n\vec{u}}{\partial t} + \nabla \cdot (n\vec{u}\vec{u}) = -\nabla \cdot P + \mu \nabla^2 \vec{u} + \vec{F}_b \qquad (3)$$

where θ_M is called mobility, μ_ϕ is the chemical potential, P is the pressure tensor, $\vec{F}_b$ is the body force, and n, ϕ are defined as

$$n = \frac{\rho_A + \rho_B}{2}, \phi = \frac{\rho_A - \rho_B}{2}$$

where ρ_A and ρ_B are the density of fluid A and fluid B respectively.

Under the lattice Boltzmann framework, Eq. (1) can be solved by iterating the evolution equation for a set of distribution functions. These distribution functions evolve with a modified lattice Boltzmann equation and BGK approximation,

$$g_i(x + e_i\delta t, t + \delta t) = g_i(x,t) + \Omega_i + (1-q)\delta g_i$$

with

$$\Omega_i = \frac{g_i^0(x,t) - g_i(x,t)}{\tau_\phi}$$

$$\delta g_i = g_i(x + e_i\delta t, t) - g_i(x,t) \qquad (4)$$

where g_i is the distribution function, Ω_i is the collision term, τ_ϕ is the dimensionless single relaxation time, e_i is the lattice velocity, and q is a constant coefficient.

In Eq. (3), the term $\nabla \cdot P$ is related to the surface tension force. This force can be rewritten as a potential term,

$$\vec{F}_s = -\nabla \cdot P = -\phi \nabla \mu_\phi - \nabla p_0$$

where $p_0 = nc_s^2$, c_s is the speed of sound.

The potential form for the surface tension force is adopted to keep the energy conservation. Mathematically, the potential form and stress form are identical. However, numerically, the discretization error is different[4]. Thus, it is useful to eliminate spurious currents.

The lattice Boltzmann implementation of Eqs. (2) and (3) can be described as

$$f_i(x + e_i\delta t, t + \delta t) = f_i(x,t) + \Omega_i \qquad (5)$$

with

$$\Omega_i = \frac{f_i^0(x,t) - f_i(x,t)}{\tau_n} +$$

$$(1 - \frac{1}{2\tau_n})\frac{w_i}{c_s^2}[(\vec{c}_i - \vec{u}) + \frac{(\vec{c}_i \cdot \vec{u})}{c_s^2}\vec{c}_i](-\phi \nabla \mu_\phi + \vec{F}_b)\delta t$$

The equilibrium distributions satisfy the conservation laws as

$$\phi = \sum_i g_i, n = \sum_i f_i$$

$$\vec{u} = [\sum_i f_i \vec{c}_i + \frac{1}{2}(-\phi \nabla \mu_\phi + \vec{F}_b)]/n$$

The details are Ref. [4].

The chemical potential is chosen as

$$\mu_\phi = A(4\phi^3 - 4\phi^{*2}\phi) - \kappa\nabla^2\phi$$

Following the same procedure as [4], we can obtain the profile along the normal direction of the interface

$$\phi = \phi^* \tanh(2\zeta / w)$$

Where ζ is the coordinate which is perpendicular to the interface, and w is the thickness of the interface layer,

$$w = \frac{\sqrt{2\kappa / A}}{\phi^*}$$

For a flat interface, the surface tension coefficient can be evaluated by Rowlinson and Widom[5].

$$\sigma = \int \kappa \left(\frac{\partial \phi}{\partial \zeta} \right)^2 d\zeta$$

We can obtain the surface tension coefficient as

$$\sigma = \frac{4\sqrt{2\kappa A}}{3} \phi^{*3}$$

Where $\phi^* = \frac{\rho_H - \rho_L}{2}$.

2.2 Wetting boundary condition

When a liquid-gas interface meets a solid wall, the angle(θ_w) is determined by the liquid-gas, solid-liquid and solid-gas surface tensions according to Young's equation

$$\cos\theta_w = \frac{\sigma_{sg} - \sigma_{sl}}{\sigma_{\mathrm{lg}}}$$

Briant et al.[3] defined the wetting boundary conditions which reproduce Young's equation in an equilibrium state. The solid-gas and solid-liquid surface tensions will be related to an additional term in the Landau free energy functional which describes the interactions at the surface between the solid and the fluid. The total free energy of the domain is obtained,

$$\psi = \psi_b + \psi_s = \int [\psi(\phi) + \frac{\kappa}{2}(\nabla\phi)^2] dn - \gamma\phi_s$$

Minimizing this Eq. with a natural boundary condition by a variational calculus, two conditions are obtained[3]. Therefore, the following wetting boundary conditions are imposed on Eq. (4). For example, at y=0,

$$\frac{\partial \phi}{\partial y} = -\frac{\gamma}{\kappa}$$

The wetting potential γ is calculated analytically by Briant et al.[3].

2.3 Results

The static contact angle of a droplet on a wall is calculated by using the present method. A hemisphere droplet with radius R placed on a wall. The bounce back boundary condition is used on all the walls, and the wetting potential γ is given on the bottom wall. Fig. 1 shows the results with the different contact angles. The droplet spreads as time passes, and finally reaches an equilibrium shape with different contact angles 46°, 90° and 134°. The present results are in good agreement with the theoretical curve obtained by Young's equation.

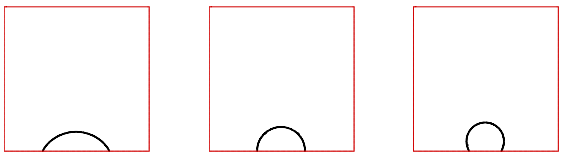

Fig. 1. The equilibrium shape with the contact angles, $\theta_w = 46^\circ, 90^\circ, 134^\circ$
(w=2, d=4, Γ=40, density ratio=1000, $\sigma = 1$).

3. Conclusion

The lattice Boltzmann method for two phase flows has been applied to the simulations of wetting dynamics by using the wetting boundary condition. The static contact angles obtained through the simulation were found to be in good agreement with Young's equation. Also, it can be easily implemented for the three dimensional case.

REFERENCES

[1] Dieter A, Wolf-Gladrow, Lattice Gas Celluar Automata and Lattice Boltzmann method, Springer: Berlin, 2000.
[2] P. Seppecher, Moving contact lines in the Cahn-Hilliard theory, Int. J. Engng Sci, Vol. 34, pp. 977-992, 1996.
[3] A. J. Briant, P. Papatzacos, P. and J. M. Yeomans, Lattice Boltzmann Simulations of Contact Line Motion in a Liquid-Gas System, Philos. T. Roy. Soc. A, Vol. 360, pp. 485-495, 2002.
[4] H. W. Zheng, C. Shu, and Y. T. Chew, A lattice Boltzmann model for multiphase flows with large density ratio, J. Comput. Phys., Vol. 218, pp. 353-371, 2006.
[5] J. S. Rowlinson, and B. Widom, Molecular Theory of Capillarity, Clarendon, Oxford, 1989.