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ON CONTACT WETTING ANGLES IN THE LATTICE BOLTZMANN METHOD AND THEIR MEASUREMENT

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Abstract Lattice Boltzmann method is applied for the computer simulation of liquid droplets that are in contact with a solid surface. In such problems, the value of contact angle at the three-phase contact line needs to be set. To achieve this, interaction forces between fluid and solid are introduced. The simulation of the equilibrium shapes of droplets is performed. We show that the use of commonly accepted forms of the interaction between fluid and solid in LBM leads to a non-physical change of the density near the solid surface. This hinders the correct calculation of heat fluxes. A new method is proposed to control the contact angles where only the tangential components of forces acting on fluid from solid nodes are taken into account (tangential force method, TFM). Use of this method does not change the fluid density in layers adjacent to the boundary. This is important in the simulation of flows with heat transfer and electrohydrodynamic flows. The dependence of the contact angle on the parameter of fluid-solid interaction is obtained.

Key words: droplets, wettability, contact angle, liquid films, lattice Boltzmann method, dielectric liquids, electric field.

AMS Mathematics Subject Classification: 76-10, 76M28.

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1 Introduction

Surface wetting and corresponding values of contact angles are important for the behavior of liquid droplets and films on a solid surface. These values depend both on the properties of the liquid and on the properties of the surface.

Processes of wetting play an important role in the technologies of cooling of solid surfaces, particularly, in microelectronics. It is known that significant heat exchange occurs in the vicinity of contact lines [1, 2, 3, 4, 5].

The degree of surface wetting is also important in the manipulating the droplets with an electric field [6, 7], and in the process of the perforation of liquid films by a non-uniform electric field [8, 9].

Presently, the lattice Boltzmann equation method (LBE, LBM) is widely used for simulating the flows of viscous liquid with phase transitions. This method is a relatively new mesoscopic approach to describe complex fluid flows [10, 11]. Modern variants of LBM compete successfully with traditional CFD methods (finite-difference, finite-element, and spectral methods). In some areas (multiphase and multicomponent flows), the lattice Boltzmann method has significant advantages. In present, LBM is widely

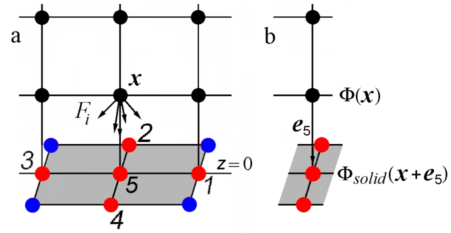

Figure 1: Interaction forces between fluid and four nearest solid nodes.

used for the simulation of multiphase fluid flows containing liquid, gas and solid phases, including the simulation of droplets and films on a substrate.

2 Surface wetting

For simulating the wetting of solid surfaces in the lattice Boltzmann method, the approaches are commonly used where the interaction forces are introduces between a fluid node (containing liquid or vapor) near the wall and nearest solid nodes. These approaches can be divided into two groups.

In the models of the first group (Fig. 1), either the effective density in solid nodes is specified [12], or the values of the pseudopotential U corresponding to this density are used [13] in the same formula as for the fluid-fluid interaction

$$\mathbf{F}(\mathbf{x}) = B\Phi(\mathbf{x}) \sum_{j=1}^{k} w(\mathbf{e}_j)\Phi_{solid}(\mathbf{x}+\mathbf{e}_j)\mathbf{e}_j. \tag{1}$$

The function Φ depends on the equation of state $P = P(\rho, T)$ of the fluid

$$\Phi(\mathbf{x}) = \sqrt{-U(\mathbf{x})} = \sqrt{\rho T_c - P(\rho, T)}. \tag{2}$$

Here, ρ is the fluid density, T is the temperature, $T_c = h^2/(3\Delta t^2)$ is the kinetic temperature of LBM pseudoparticles. The value of Φ_{solid} in a boundary node is equal to the value of Φ in the nearest fluid node. The parameter B determines the wetting of a boundary, $B = 1$ corresponds to the neutral wetting.

In the second group of models [14], the total force consists of two parts. The first one provides the neutral wetting in the same way, as in the previous case. Also, additional interaction forces with the nearest solid nodes are introduced (Fig. 1) by the formula

$$\mathbf{F}(\mathbf{x}) = \beta\Phi^2(\mathbf{x}) \sum_{j=1}^{k} w(\mathbf{e}_j)s(\mathbf{x}+\mathbf{e}_j)\mathbf{e}_j. \tag{3}$$

The indicator function s takes the value $s = 1$ in solid nodes, and $s = 0$ in fluid ones. The interaction (adhesion) parameter $\beta = 0$ corresponds to the neutral wetting.

Figs. 2a,c and 3a,c show the simulation results with the model (1). The drawback of this method is that the density in a thin layer adjacent to the boundary changes when the degree of wetting changes (Figs. 2c and 3c). This hinders the correct calculation of heat fluxes. Use of the model (3) produces similar profiles of density near the surface.

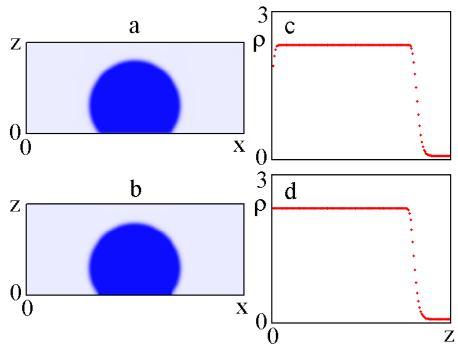

Figure 2: (a),(b) – Fluid density in central vertical section of droplet at poorly wetting surface (contact angle $\theta \approx 120°$). (c),(d) – Fluid density graphs along the vertical droplet axis. (a),(c) – Calculation with model (1); (b),(d) – calculation with tangential force method (4)–(5). Bond number is $\mathrm{Bo} = \rho g r^2/\sigma \approx 0$ (ρ is the liquid density, r is the droplet radius, g is the gravity acceleration, σ is the surface tension). Lattice size $384 \times 384 \times 160$.

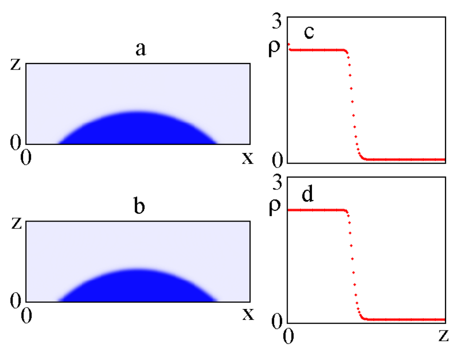

Figure 3: (a),(b) – Fluid density in central vertical section of droplet at well-wetting surface (contact angle $\theta \approx 49°$). (c),(d) – Fluid density graphs along the vertical droplet axis. (a),(c) – Calculation with model (1); (b),(d) – calculation with tangential force method (4)–(5). Bond number is $\mathrm{Bo} \approx 0$. Lattice size $400 \times 400 \times 144$.

In the works [15, 16], an idea of a new class of methods to control contact angles was proposed which are free of this drawback. In addition to the neutral wetting for $B = 1$ in Eq. (1), only tangential components of forces acting on the fluid in liquid nodes from nearest-neighbor solid nodes (Fig. 4) are introduced (tangential force method, TFM). For the three-dimensional model D3Q19, the formulas are

$$F_x(\mathbf{x}) = -\beta\Phi(\mathbf{x}) \sum_{j=1}^{4} \Phi_{solid}(\mathbf{x} + \mathbf{e}_j) e_{jx}. \tag{4}$$

$$F_y(\mathbf{x}) = -\beta\Phi(\mathbf{x}) \sum_{j=1}^{4} \Phi_{solid}(\mathbf{x} + \mathbf{e}_j) e_{jy}. \tag{5}$$

These forces are directed along the solid surface. The interaction parameter $\beta = 0$ corresponds to the neutral wetting, $\beta > 0$ leads to hydrophilic surfaces, and $\beta < 0$ – to

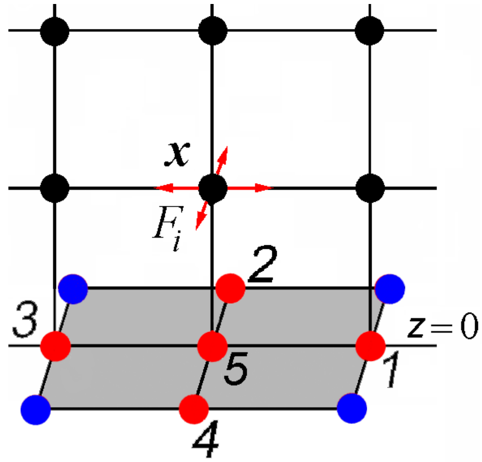

Figure 4: Additional tangential forces F_x, F_y.

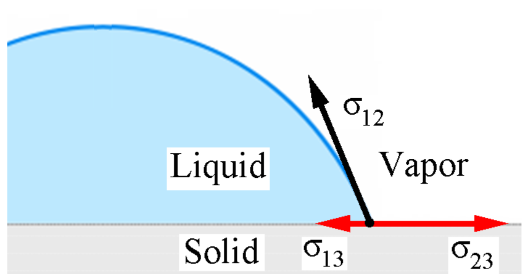

Figure 5: Young's law for the surface tension forces at the triple-phase contact.

hydrophobic ones. These tangential interaction forces in the nodes adjacent to a wall are applied only in the transition layer liquid-vapor where the fluid density lies in the range from $(\rho_l + \rho_{vap})/2$ to $0.9\rho_l$. Here, ρ_l is the density of the liquid, and ρ_{vap} is the density of the saturated vapor for the given temperature.

In this case, horizontal forces have the well-known meaning of the surface tension in the vertex of the contact wetting angle (Fig. 5) according to the classic Young's law [17, 18]

$$\cos\theta = \frac{\sigma_{23} - \sigma_{13}}{\sigma_{12}}. \tag{6}$$

Here, σ_{12} is the surface tension of liquid, σ_{23} is the surface energy at the boundary between solid and vapor, and σ_{13} is the surface energy at the boundary between solid and liquid.

3 Contact angle measuring

In simulations of droplets placed on a flat surface, the values of the contact angle need to be measured for different values of the parameter β. In the simplest case of the zero gravity (when droplet surface is spherical), the contact angle is determined by the formula (Fig. 6)

$$\theta = 2\arctan(H/G). \tag{7}$$

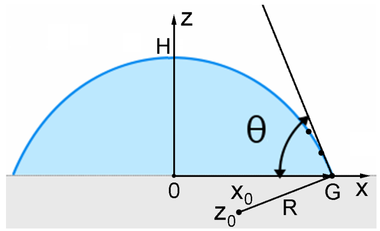

Figure 6: Radius of inscribed circle R and contact angle θ.

Here, H is the height of the droplet, and G is the radius of the wetting spot. The boundary of the droplet is defined as the surface where the fluid density is equal to $\rho = (\rho_l + \rho_{vap})/2$. In the case of a non-spherical droplet shape (gravity is not negligible), more complicated formulas are necessary. For instance, the coordinates of the center of the inscribed circle x_0 and z_0, and its radius R can be calculated using the last three boundary points. Then, the wetting angle can be found by the formula

$$\tan\theta = (G - x_0)/|z_0|. \tag{8}$$

In the known tangential method, a tangent is drawn through the last two points, and the differences of their coordinates Δx and Δz are used

$$\theta = \arctan(\Delta z/\Delta x). \tag{9}$$

The results become more accurate, if a correction for the radius of the inscribed circle is taken into account [19]

$$\theta = \arctan(\Delta z/\Delta x) + \Delta l/(2R). \tag{10}$$

Here, $\Delta l = \sqrt{\Delta x^2 + \Delta z^2}$ is the length of the chord between the last two points.

A local approximation by the parabola passing through the last three points $x = a + bz + cz^2$ is also possible. In this case,

$$\tan\theta = \left.\frac{dz}{dx}\right|_{z=0}. \tag{11}$$

When the gravity is practically absent, the droplet has a spherical shape. The values of contact angles determined by different methods for neutral wetting are presented in the Table 1.

It can be seen that even in this simplest case, there is a scatter of the angle determined by different methods. The error in this case for the methods (7), (8), (10), and (11) can be estimated as $\pm 1°$.

4 Simulation results

Figs. 2b,d and 3b,d show the results of the simulation of droplets using the method of tangential forces according to Eqs. (4)–(5). For a poorly-wetting surface (Fig. 2b,d), the value of the adhesion parameter is $\beta = -0.8$ which leads to the contact angle of

Table 1: Measured values of contact angles for the case of neutral wetting $\beta = 0$. Bond number is equal to 0.001.

Measurement method	Time		
	$t = 15000$	$t = 17000$	$t = 20000$
"Hemispherical" geometry (7)	90.65°	90.64°	90.63°
Line through two points (9)	87.19°	87.31°	87.22°
Two points with correction (10)	89.47°	89.70°	89.55°
Inscribed circle (8)	89.12°	89.36°	89.22°
Parabola (11)	89.15°	89.40°	89.26°

$\theta \approx 120°$. For a well-wetting surface (Fig. 3b,d), the values are $\beta = 0.7$ and $\theta \approx 49°$. The parasitic liquid density change in a thin layer adjacent to the boundary is absent in both cases (Figs. 2d and 3d)).

Fig. 7 presents the results of the simulation with the method of tangential forces of droplets at solid surfaces with different wetting angles in the presence of gravity.

The dependence of contact angle measured by the formula (10) on the parameter β is shown in Fig. 8. It is clearly seen that the value of the contact angle can be controlled by changing the interaction parameter β. The accuracy of the contact angle measurements by different methods (8), (10), and (11) corresponds roughly to the range of $\pm 4°$ which is explained by the discreteness of the calculation lattice.

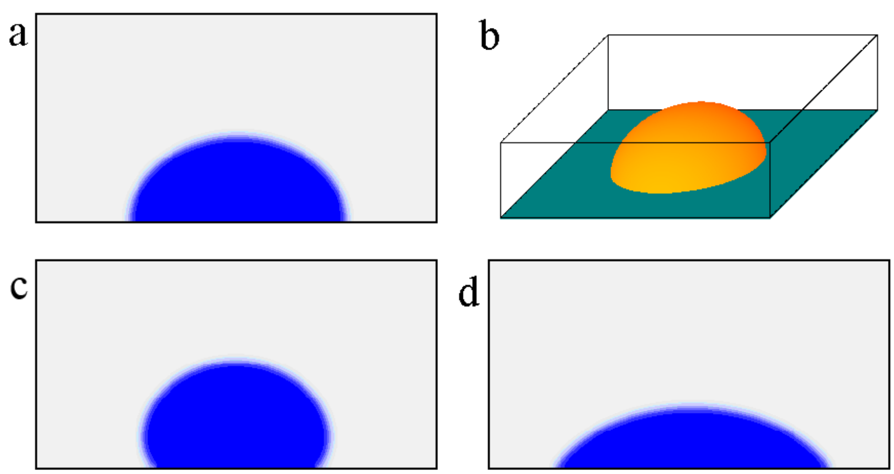

Figure 7: Droplets of the same volume on a solid surface with different contact angles. (a),(b) – neutral wetting $\beta = 0$, contact angle $\theta = 90°$. (c) – hydrophobic surface $\beta = -1$, contact angle $\theta = 122°$. (d) – hydrophilic surface $\beta = 0.5$, contact angle $\theta = 63°$. Bond number is equal to 2.1(a), 1.5(c), 7.2(d).

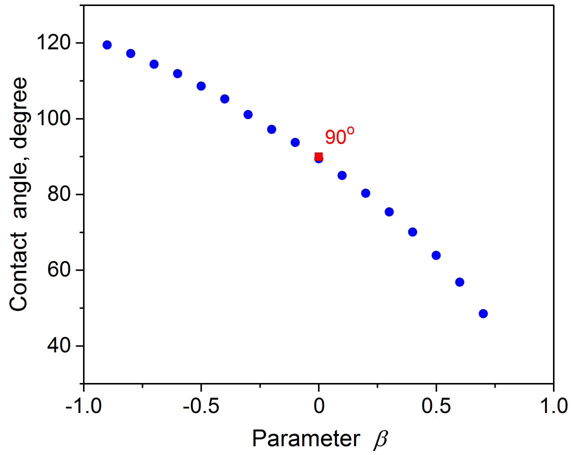

Figure 8: Contact angle dependence on the parameter β for the tangential force method.

5 Conclusion

The equilibrium shape of droplets on a solid surface is simulated using the lattice Boltzmann method. We show that the use of commonly accepted forms of the interaction between fluid and solid in LBM leads to a non-physical change of the density near the surface that hinders the correct calculation of heat fluxes.

A new method is proposed to control the contact angles where only the tangential components of additional forces acting on fluid from solid nodes are taken into account (tangential force method, TFM). Use of this method keeps the density in the layers adjacent to the boundary, which is important in the simulation of flows with heat transfer and electrohydrodynamic flows. The dependence of the contact angle on the parameter of fluid-solid interaction is obtained.

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