Droplet Flow Along the Wall of Rectangular Channel with Gradient of Wettability

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Abstract. The lattice Boltzmann equations (LBE) method (LBM) is applicable for simulating the multiphysics problems of fluid flows with free boundaries, taking into account the viscosity, surface tension, evaporation and wetting degree of a solid surface. Modeling of the nonstationary motion of a drop of liquid along a solid surface with a variable level of wettability is carried out. For the computer simulation of such a problem, the three-dimensional lattice Boltzmann equations method D3Q19 is used. The LBE method allows us to parallelize the calculations on multiprocessor graphics accelerators using the CUDA programming technology.

INTRODUCTION

A drop lying on a horizontal solid surface is immovable. However, if the properties of the surface material change along the coordinate, the wettability level can also change. This can be achieved by gradient coatings. In this case, contact angles also vary in coordinate. Therefore, the drop can no longer be in equilibrium and begins to move.

The wetting angle is closely related to the magnitude of the interaction forces between the liquid molecules and the solid surface. In general, the contact angles also depend on the velocity of the contact line along the surface.

For a non-stationary motion of a drop, the problem should be modeled only numerically. In this case, it is necessary to describe fluid flows with surface tension at the liquid-gas interface and interaction with a solid surface. For the computer simulation of such a problem, the lattice Boltzmann equations method (LBM), first proposed in [1,2], is used.

LATTICE BOLTZMANN METHOD

For the computer simulation of such a problem, the variant of the lattice Boltzmann equation method (LBM), described in [3-8], was used. For the three-dimensional model D3Q19 [9], 19 possible particle velocity vectors $\mathbf{c}_k$ are allowed, for which the values of velocity modulus are assumed to be $|\mathbf{c}_k| = 0$, $h/\Delta t$ or $\sqrt{2}h/\Delta t$, where h is the grid spacing, and Δt is the time step. Then, the evolution equation for the distribution functions N_k can be written in the form

$$N_k(\mathbf{x}+\mathbf{c}_k\Delta t, t+\Delta t) = N_k(\mathbf{x},t) + \Omega_k(N) + \Delta N_k \ , \qquad (1)$$

where $\Omega_k = (N_k^{eq}(\rho,\mathbf{u}) - N_k(\mathbf{x},t))/\tau$ is the collision operator in the form of BGK, τ is the characteristic relaxation time to local equilibrium. The dimensionless relaxation time τ defines the kinematic viscosity $\nu = \theta(\tau - 1/2)\Delta t$. To account for the volume forces (internal and external), the Exact Difference Method (EDM) is used [6-8]

$$\Delta N_k(\mathbf{x},t) = N_k^{eq}(\rho,\mathbf{u}+\Delta\mathbf{u}) - N_k^{eq}(\rho,\mathbf{u}) \ . \qquad (2)$$

XV All-Russian Seminar "Dynamics of Multiphase Media" (DMM2017)
AIP Conf. Proc. 1939, 020046-1–020046-6; https://doi.org/10.1063/1.5027358
Published by AIP Publishing. 978-0-7354-1631-4/$30.00

Here, the value of the velocity after the action of the force $\mathbf{F}$ during the time step is equal to $\mathbf{u}+\Delta\mathbf{u}=\mathbf{u}+\mathbf{F}\Delta t/\rho$. The values of equilibrium distribution functions N_k^{eq} are calculated as [10]

$$N_k^{eq}(\rho,\mathbf{u})=\rho w_k\left(1+\frac{\mathbf{c}_k\mathbf{u}}{\theta}+\frac{(\mathbf{c}_k\mathbf{u})^2}{2\theta^2}-\frac{\mathbf{u}^2}{2\theta}\right). \tag{3}$$

Here $\theta=(\Delta x/\Delta t)^2/3$ is the "kinetic temperature of LBE pseudo-particles. For the model D3Q19, the weight coefficients are equal to $w_0=1/3$, $w_{1-6}=1/18$ and $w_{7-18}=1/36$ [9]. The fluid density ρ and velocity $\mathbf{u}$ at the node are calculated by the formulas

$$\rho=\sum\nolimits_{k=0}^{b}N_k\ , \tag{4}$$

$$\rho\mathbf{u}=\sum\nolimits_{k=1}^{b}\mathbf{c}_kN_k\ . \tag{5}$$

The physical velocity of fluid should be calculated at half time step [11] as $\mathbf{u}_*=\mathbf{u}+\Delta\mathbf{u}/2$.

To describe the equation of state (EOS) in the form $P(\rho,T)$, the pseudopotential model [12] is used in which internal forces $\mathbf{F}=-\nabla U$ acting on the substance at the lattice nodes are introduced. Here, $U=P(\rho,T)-\rho\theta$ is the pseudopotential. The numerical approximation of the gradient of the pseudopotential is very important. In [3,4], Kupershtokh et al. proposed the isotropic finite-difference approximation of the gradient operator that can be written in vector form as

$$\mathbf{F}(\mathbf{x})=\frac{1}{bh}\left[(1-2A)\Phi(\mathbf{x})\sum_k\frac{G_k}{G}\Phi(\mathbf{x}+\mathbf{e}_k)\mathbf{e}_k+A\sum_k\frac{G_k}{G}\Phi^2(\mathbf{x}+\mathbf{e}_k)\mathbf{e}_k\right]. \tag{6}$$

The function Φ was specially defined as

$$\Phi^2=-U=\rho c_s^2-p(\rho,T)\,. \tag{7}$$

Note, the pseudo-potential $U<0$ in the region of stability of calculations [8]. For three-dimensional model D3Q19, the values of coefficients are different for basic directions $G_k=G$ and for diagonal directions $G_k=G/2$ to ensure the isotropy of space. The value of the coefficient $b=3$ for D3Q19 model. In particular cases, the "combined" approximation (6) becomes "mean value" approximation [12] for $A=0.5$ and "local" approximation [13] for $A=0$ [4]. This so-called "combined" approximation was compared in [3,4] with "local" and "mean-value" approximations. The "combined" approximation is more stable and allow one to reach the values of density ratio up to 10^6 for quasi-stationary flat liquid-vapor interface.

We used the van der Waals equation of state written in the reduced variables

$$\tilde{P}=\frac{8\tilde{\rho}\tilde{T}}{3-\tilde{\rho}}-3\tilde{\rho}^2\ . \tag{8}$$

Here, $\tilde{p}=p/p_{\rm cr}$, $\tilde{\rho}=\rho/\rho_{\rm cr}$, $\tilde{T}=T/T_{\rm cr}$ are the reduced variables, $p_{\rm cr},\rho_{\rm cr},T_{\rm cr}$ are the pressure, density and temperature at the critical point. The value $A=-0.152$ was obtained in [4] for van der Waals EOS as the optimal value for which the coexisting curve (binodal curve) simulated by LBM coincides best with the theoretical results (Maxwell curve).

The effect of a solid surface on the fluid is simulated by the forces of interaction between the fluid and solid surface nodes, which describe the degree of wetting and the magnitude of the contact angles. These forces act on the node $\mathbf{x}$ belonging to the fluid from the side of the nearest nodes representing a solid surface (see Fig. 1). The simple model for these forces has the form [14, 15]

$$\mathbf{F}_k(\mathbf{x})=Bw_k\tilde{\rho}(\mathbf{x})\,\tilde{\rho}_{\rm eff}(\mathbf{x}+\mathbf{e}_k)\,\mathbf{e}_k\ . \tag{9}$$

Here, $\tilde{\rho}_{\rm eff}$ is the effective reduced density of solid surface, B is the parameter of interaction. In fact, only the product $B\tilde{\rho}_{\rm eff}$ determines the forces and, accordingly, the wettability level and the value of the contact angle.

The shapes of static drops on the solid wall at the different values of wettability parameter are shown in Fig. 2. For the temperature $\tilde{T}=0.7$, $B=0.374$ and $\tilde{\rho}_{\rm eff}=1$, the static contact angle α is equal to $\approx 90^\circ$ (see Fig. 3). Thus, contact angles are not prescribed in lattice Boltzmann method but are simulated in natural way.

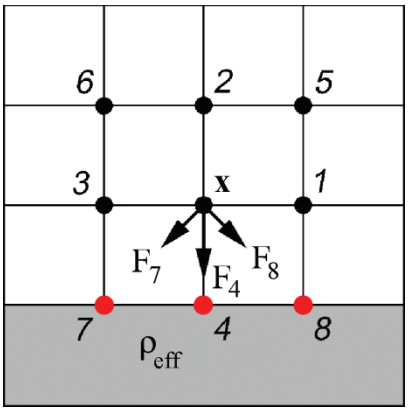


FIGURE 1. Interaction forces $F_k(\mathbf{x})$ between fluid and solid wall

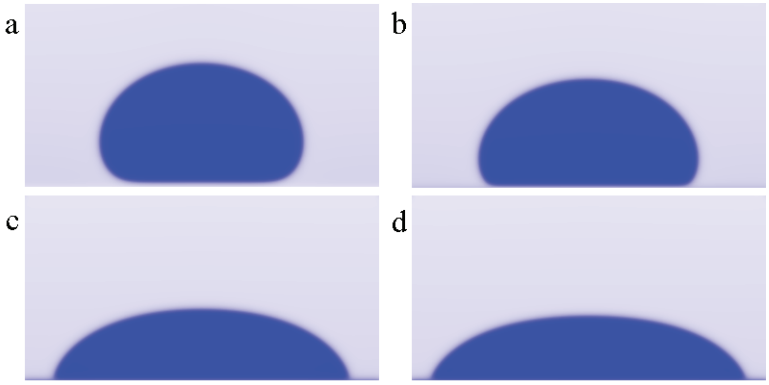


FIGURE 2. The shapes of static drops on the solid wall at the different levels of wettability

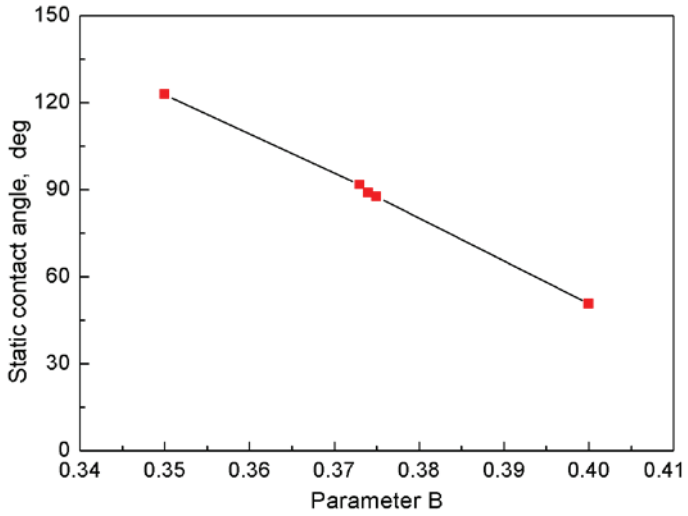


FIGURE 3. Static contact angle α for drops on horizontal solid partly wettable surface vs. parameter of interaction B. $\tilde{T} = 0.7$, $\tilde{\rho}_{\text{eff}} = 1$

PARALLEL GPU CALCULATIONS

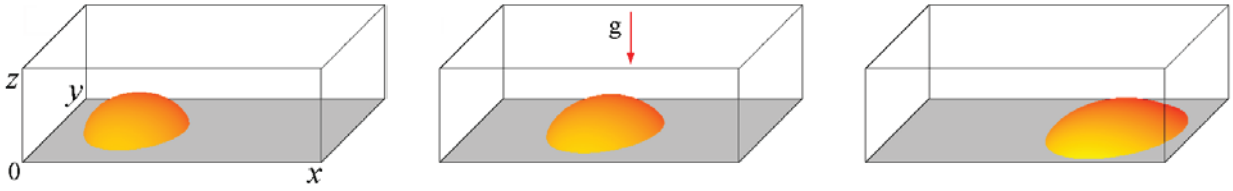
The calculations are carried out on a supercomputer "Supermicro 4027GR" based on graphics processors (GPU) (6 GTX Titan-Black modules and 2 GTX Titan-Xp modules). The total number of available stream processors (cores) of the computer is more than 30,000. Parallel calculations are performed simultaneously on all cores of several GPUs depending on a specific problem solved. The total amount of fast internal memory in GPUs is 60 GB. The internal memory of the GPU is an order of magnitude faster than the computer's RAM. For parallel programming we use the CUDA (Compute Unified Device Architecture) technology.

THE RESULTS OF COMPUTER SIMULATIONS

The results of the three-dimensional modeling of a drop moving along a horizontally partly wettable wall of the rectangular channel with a wetting gradient are shown in Fig. 4. The dependence of the effective reduced density on the coordinate is assumed to be linear

$$\tilde{\rho}_{\text{eff}} = 0.95 + 0.00037x \ . \qquad (10)$$

The non-slip boundary conditions were taken on the solid wall $z = 0$. For this purpose we use the well-known and quite simple “bounce-back” rule. The periodic boundary conditions were in y direction.



(a) (b) (c)

FIGURE 4. Droplet flow along rigid surface with variable wettability (10). Lattice size is 512×272×160.
$\tilde{T} = 0.7$. $t =$ 2000 (a), 20000 (b), 50000 (c)

The boundary of the central vertical section ($y = 136$) of a moving drop (Fig. 5) was obtained by computer processing of the density field of matter in this section (Fig. 6). The motion of the droplet along the x axis arises because the advancing contact angle α_{ad} is less than the receding one α_{re}, since the degree of wettability increases with increasing coordinate x in accordance with (10). In this case, the relation is satisfied $\cos\alpha_{\text{ad}} > \cos\alpha_{\text{re}}$.

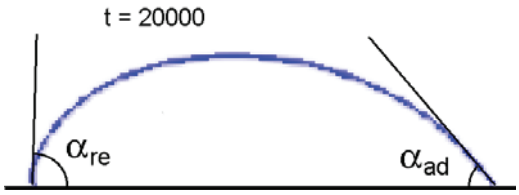


FIGURE 5. The boundary of a moving drop in the central vertical section $y = 136$. $t =$ 20000

(a) (b) (c)

FIGURE 6. The density distribution for the moving drop in the central vertical section $y = 136$.
$t =$ 2000 (a), 20000 (b), 50000 (c)

The coordinates of the leading (x_2) and trailing (x_1) edges of contact line for the drop moving on the horizontal surface with the gradient of wettability are shown in Fig. 7. As the droplet moves to the area of increased wettability, its height decreases.

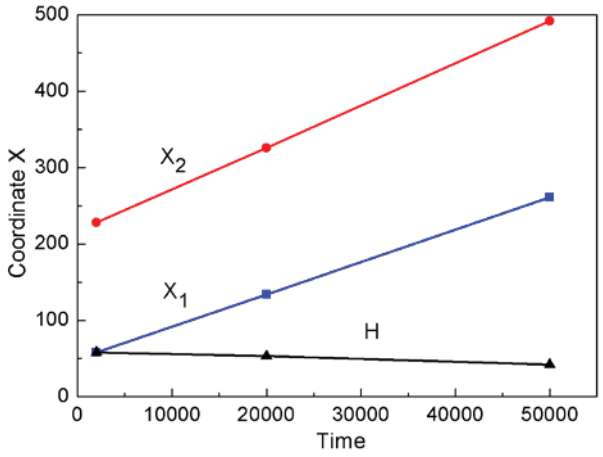


FIGURE 7. The coordinates of the leading (x_2) and trailing (x_1) edges of contact line of the moving drop. The drop height H

A dimensionless number that characterizes the importance of gravitational forces compared to surface tension forces is the Bond number

$$\mathrm{Bo} = \frac{\rho g H^2}{\sigma} . \tag{11}$$

The Bond number in dimensionless variables has the form

$$\mathrm{Bo} = \frac{\tilde{\rho}\tilde{g}\tilde{H}^2}{k\tilde{\sigma}} . \tag{12}$$

Here, the dimensionless coefficient

$$k = \frac{p_{\mathrm{cr}}}{\rho_{\mathrm{cr}}}\left(\frac{\Delta t}{h}\right)^2 \tag{13}$$

introduced in [4,8] plays an important role in the stability of simulations. For reasonable choice $h/\Delta t \sim 10^3$ m/s, we have the value $k \sim 0.01$ for argon and for some other fluids. For simulations shown above, the temperature is $\tilde{T} = 0.7$, the density is $\tilde{\rho} = 2.14$, the surface tension is $\tilde{\sigma} = \sigma/(p_{\mathrm{cr}}h) = 3.3$ [14], the initial height of drop is $\tilde{H}_0 = 55$, the value of gravity $\tilde{g} = g\Delta t^2/h = 0.000005$. Hence, the Bond number is equal to $\mathrm{Bo} \approx 1$.

The ratio of the magnitude of the viscous friction forces on a solid surface to the capillary forces is defined by capillary number

$$\mathrm{Ca} = \frac{\nu\rho V}{\sigma(\cos\alpha_{\mathrm{ad}} - \cos\alpha_{\mathrm{re}})} . \tag{14}$$

For dimensionless variables we have

$$\mathrm{Ca} = \frac{\tilde{\nu}\tilde{\rho}\tilde{V}}{k\tilde{\sigma}(\cos\alpha_{\mathrm{ad}} - \cos\alpha_{\mathrm{re}})} . \tag{15}$$

For kinematic viscosity $\tilde{\nu} \approx 0.07$ and the drop velocity $\tilde{V} \approx 0.0045$, the capillary number in our simulations is $\mathrm{Ca} \sim 0.03$.

CONCLUSION

This variant of lattice Boltzmann method allows one to simulate the interfaces between liquid and vapor phases. The LBE method is applicable for simulating the multiphysics problems of flows with free boundaries, taking into account the viscosity, surface tension, evaporation and wetting degree of a solid surface.

The interaction forces between nodes of fluid and rigid wall define the degree of wetting and the magnitudes of the contact angles.

Modeling of the nonstationary motion of a drop of liquid along a solid surface with a variable level of wettability is carried out. The initial spreading of a drop over the surface is determined by the Bond number Bo. The speed of the droplet motion along the surface is related to the dimensionless parameter Ca (the capillary number).

The LBE method can be easily parallelized on multiprocessor graphics accelerators using the CUDA programming technology.

ACKNOWLEDGMENTS

This work was carried out in part in accordance with the project III.22.3.1.

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