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Contact angle measurement in lattice Boltzmann method

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ABSTRACT

Contact angle is an essential characteristic in wetting, capillarity and moving contact line; however, although contact angle phenomena are effectively simulated, an accurate and real-time measurement for contact angle has not been well studied in computational fluid dynamics, especially in dynamic environments. Here, we design a geometry-based mesoscopic scheme for on-the-spot measurement of the contact angle in the lattice Boltzmann method. The measuring results without gravity effect are in good agreement with the benchmarks from the spherical cap method. The performances of the scheme are further verified in gravitational environments by simulating sessile and pendent droplets on smooth solid surfaces and dynamic contact angle hysteresis on chemically heterogeneous surfaces. This scheme is simple and computationally efficient. It requires only the local data and is independent of multiphase models.

1. Introduction

Contact angle, which indicates the wettability of a solid surface by a liquid, is a characteristic quantity in a great amount of wonderfully natural phenomena and significantly industrial applications, such as capillarity, microfluidics, nanotechnology, moving contact line, coating technology, etc [1,2]. Essentially, both of the static and dynamic contact angles should be measured at contact line on the microscale [1]. Experimenters have developed all kinds of methods to determine contact angle. Bigelow et al. set up the most widely used technique, which utilized a telescope-goniometer to directly measure the tangent angle at the three-phase contact point on a sessile droplet profile [3]. Angles measured in such a way are often quite close to advancing contact angles. Equilibrium contact angles can be obtained through the application of well-defined vibrations [4]. Extrand and Kumagai studied the contact angle hysteresis on a variety of polymer surfaces by using an inclined plate method, in which a sessile droplet locates on an inclined plate and both of the advancing and receding contact angles are simultaneously obtained [5]. Kwok et al. used a motor-driven syringe to control the rate of liquid addition and removal to study advancing, receding, or dynamic contact angles [6]. Besides observing a sessile droplet on a solid sample, a telescope-goniometer is also necessary in other contact angle measurements. The captive bubble method forms an air bubble beneath the solid sample, which is immersed in the testing liquid [7]. The contact angle formed by the air bubble in liquid can also be directly measured. The tilting plate method applies a solid plate with one end immersed in the liquid and forms a meniscus on both sides of the plate [8]. The plate inclines slowly until the meniscus becomes horizontal on one side of the plate and then the angle between the plate and the horizontal is the contact angle. It is generally recognized that the direct measurement

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of drop contact angles with a telescope-goniometer can yield an accuracy of approximately ±2° [9]. The Wilhelmy balance method is another type of popular scheme to measure contact angle [10]. A solid sample is manipulated to immerse into or emerge from the wetting liquid. The task of measuring an angle is reduced to the measurements of the weight and length, which can be performed with high accuracy and without subjectivity. The method is also suitable to measure dynamic contact angle and hysteresis, because the three-phase line can be in wholesale motion assuring achievement of maximal advancing and minimum receding contact angles [11]. The experimental measurements of the contact angle promote to investigate the surface tensions and wetting mechanisms of the solid surfaces, especially interpretation of contact angles in terms of surface energetics of solids [9].

Numerical simulation has been developed into an effective way to research fluid flow and is expected to provide more rich details than experiments. In computational fluid dynamics, there are usually several methods available to measure a contact angle. The measurement of the drop image by a goniometer is relatively rough and subjective after the images are generated from the simulation data [12]. In a more accurate way, a graphical analysis can be applied to obtain the contact angle from the image [13]. Since the fluid images have to be exported before the measurement, these methods are time-consuming and cannot serve as an on-the-spot measurement. Ignoring the gravity effect, a droplet holds a perfect spherical cap on a horizontal solid surface owing to the surface tension. The contact angle can be accurately calculated based on the measurement of the height and bottom width of the droplet [14,15]. This scheme is referenced here as the spherical-cap method. On chemically striped patterned surfaces, the contact line is corrugativus, the contact angle can be determined using the height of the droplet and the radius of curvature, which fits the droplet profile [16]. It is more complex in molecular dynamics simulations. Since the drop size reduces to nanoscale, there is not a steady interface between gas and liquid. The drop contours have to be fitted by a least square technique [17,18]. Although these theoretical methods are simple and easy to implement, they are limited in a zero-gravity equilibrium environment. For diffuse-interface simulations, Ding et al. proposed a geometric formulation of wetting condition based on the gradient of the volume fraction for binary fluid flows, by which the prescribed contact angle can be correctly obtained [19]. Lee et al. improved the accuracy of the contact angle boundary condition as well as its numerical stability by a characteristic interpolation [20]. Considering to the relaxation of dynamic contact angle, Dong further extended the contact-angle boundary conditions to simulate dynamic wall-bounded gas/liquid flows with large density ratio [21]. Leclaire et al. imposed the desired contact angle at the boundary as a Dirichlet boundary condition and then studied immiscible two-phase pore-scale imbibition and drainage in porous media [22,23]. As for these contact angle conditions, the main efforts were focusing on the wetting boundary constraints, but not on the evaluations of contact angles, even more not on the calculation of the dynamic contact angle. Moreover, these imposing procedures of contact-angle boundary conditions are computationally complex and nonlocal. Especially, they involve the intervention to the evolution of flow field. Therefore, a simple, exact and on-the-spot measurement of contact angle is meaningful for the numerical investigation of wetting phenomena.

Essentially, contact angle is a geometrical concept. Only for some special cases, such as a sessile droplet at zero-gravity mechanical equilibrium on a horizontal surface, the contact angle can be theoretically explained by Young's equation. In a dynamic or nonequilibrium environment, the contact angle should be measured through a geometrical method. The lattice Boltzmann method has developed into an alternative tool to model multiphase flow systems, and been successfully applied to many of the fields related to the surface wetting science and engineering application [15,24]. Its regular and mesoscopic lattices lay a foundation for efficient contact angle measurement. In this paper, we design a geometry-based mesoscopic scheme to measure the real-time contact angle. The various test cases with and without gravity are conducted to verify the proposed scheme. The computational results show that the scheme is simple, accurate and efficient.

The paper is organized as follows. In Section 2, we introduce the chemical-potential multiphase lattice Boltzmann model. Section 3 proposes the mesoscopic contact angle measurement, whose computational accuracy is verified by comparing with the benchmarks. In Section 4, a series of droplet deformations under gravity are simulated and the contact angles are measured by the proposed method. Section 5 is about the investigations of the contact angle hysteresis. Finally, Section 6 concludes the paper.

2. Chemical-potential-based multiphase model

Numerical simulation of multiphase flow is one of the most successful applications for the lattice Boltzmann method (LBM) [15,24]. Originating from the cellular automaton concept and kinetic theory, the intrinsic mesoscopic properties make LBM outstanding to model complex fluid systems involving interfacial dynamics [25–28] and phase transitions [29–37]. Discretized fully in space, time and velocity, the lattice Boltzmann equation with a single relaxation time can be concisely written as [38]

$$f_i(\boldsymbol{x} + \boldsymbol{e}_i, t + 1) - f_i(\boldsymbol{x}, t) = -\frac{1}{\tau}[f_i(\boldsymbol{x}, t) - f_i^{(eq)}(\boldsymbol{x}, t)], \tag{1}$$

where $f_i(\boldsymbol{x}, t)$ is the particle distribution function at lattice site $\boldsymbol{x}$ and time t, $\boldsymbol{e}_i$ is the discrete speeds with $i = 0, \ldots, N$, τ is the relaxation time, and $f_i^{(eq)}$ is the equilibrium distribution function

$$f_i^{(eq)}(\boldsymbol{x}, t) = \rho\omega_i[1 + 3(\boldsymbol{e}_i \cdot \boldsymbol{u}) + \frac{9}{2}(\boldsymbol{e}_i \cdot \boldsymbol{u})^2 - \frac{3}{2}u^2], \tag{2}$$