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A study on the droplet dynamic behavior on the moving flat plate in the presence of the upper flat tip

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ABSTRACT

This study carries out three-dimensional numerical simulation using the lattice Boltzmann method to investigate the dynamic behavior of the water meniscus formed between a moving flat bottom wall and a flat tip surface. The effects of the initial droplet contact angle of the bottom wall and upper tip surface, the moving velocity of the bottom wall on the dynamic behavior of the droplet are considered in this study. Under the influence of these parameters considered, the present results show the change in the shape of droplet as a function of time when the droplet is moving in between the bottom wall and the upper tip surface, and also when the droplet is moving along the bottom wall after the droplet completely escapes from the influence of the upper tip surface. This study also shows the variation of the dynamic contact angle of droplet as well as the dimensionless wet lengths between the droplet and the bottom wall or the flat tip as a function of time.

1. Introduction

A liquid bridge is formed when a liquid interconnects two different solid surfaces. This phenomenon has recently been widely used in various applications, such as lithography using atomic force microscopy (AFM) and crystal generation technology through a liquid column. The importance of liquid bridges is being increasingly recognized. Dip-pen nanolithography (DPN) is a technique for directly printing on a solid substrate using AFM. The method uses meniscuses between a tip and a solid substrate to move molecules concentrated on the AFM tip to the solid substrate. The meniscuses play the role of a liquid bridge, in which various forces affect the size of the adhesive force depending on the size of the meniscus. Such forces include the capillary force, electrostatic force, and van der Walls force [1–11].

Previous studies have focused on the meniscus mainly contacting fixed surfaces, the changes in capillary forces, and the changes in the shapes of the meniscus when changing the distances between two surfaces. Mathematical studies are currently being performed on the forces exerted on applicable meniscuses in various fields [12–17]. Chen et al. [12] performed a study on the meniscus between a fixed sphere and surface. They also performed a mathematical study on the meniscus between two spheres with different sizes. Their mathematical study has been compared with the results of experiments by Willett et al., [13] and the mathematical results coincided with experimental results. The force of the non-dimensional liquid bridge was affected by the separation distance, the volume of the liquid bridge, and the contact angle.

In meniscuses with the same volume, the force exerted on the meniscus (the liquid bridge force) decreases as the separation distance increases. In meniscuses with the same separation distance, the forces exerted on the meniscuses increase as the meniscus volume increases. De Souza et al. [14] performed a study on the capillary forces exerted on the meniscus between two surfaces. The distances between the two surfaces were very small, and the effects of contact angles between two surfaces and the meniscus were studied mathematically. When the contact angle between the two surfaces and meniscus indicates hydrophilic properties, the dimensionless force decreases as the distance between the two surfaces increases. In the case of hydrophobic properties, however, the dimensionless force increases as the distance between the two surfaces increases. The mathematical studies coincided relatively well with the results of experiments.

Recently, studies on meniscuses have been performed using numerical analysis methods, such as molecular dynamics (MD) and the lattice Boltzmann method (LBM). Numerical studies can overcome the disadvantages of mathematical and experimental studies. Jang et al. [18] studied the capillary forces of the meniscus between a hydrophilic surface and a hydrophilic or hydrophobic tip using lattice gas models under various humidity conditions. The pull-off force reached a plateau very rapidly as humidity increased when using a hydrophobic tip. When the tip was weakly hydrophilic, however, the pull-off force did not reach the

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plateau value but increased gradually. When the tip was strongly hydrophilic, the pull-off forces showed different aspects depending on the relative humidity.

Choi et al. [19] studied the changes in the shapes of a meniscus occurring between an AFM tip and a sample surface using molecular dynamics. Sharp decreases in the contact angles were observed when the surface energy was 0.5 Kcal/mol due to hydrophilic effects. When the surface energy was higher, however, there were no changes in the contact angle of the meniscus. Ko et al. [20] studied the dynamic behavior of a meniscus on a surface with nano-sized stripe patterns using molecular dynamics. They studied the effects on the dynamic behavior of the meniscus resulting from changes in the surface energy, column height, column area, and the distances between the columns. On a smooth plate, the contact angle of the meniscus decreased as the surface energy increased. Also, in a study on the changes of the contact angle according to the heights of the column, water molecules were smeared into the gaps between columns when the surface energy was 0.3 Kcal/mol or higher. The number of water molecules smeared into the gaps increased as the surface energy increased. The contact angles of the column at different areas and distances between columns follow the Cassie and Baxter equation overall.

One of the advantages of the lattice Boltzmann method is fast calculation speed and easy multi-phase analysis. Multi-phase problems have recently been used in engineering applications such as nuclear power stations, engine designs, and chemical apparatuses. Multi-phase means that the flow changes from a liquid phase to a gas phase, or the flow of fluids do not mix with each other, as with oil and water. Multi-phase problems have been studied by many researchers [21–23]. Cox [21] studied the flow of non-mixed fluids under conditions of very low capillary number (*Ca*). They compared the results of theoretical studies and experimental results. Zhou and Pozrikidis [22] studied the flow of fluid and dynamic behavior in 2-dimensional channels. The fluid flow was a pressure-driven flow, and the conditions considered were the *Ca* and the volume fraction. The droplets stopped under high *Ca* conditions but gathered around the center of the 2-dimensional channels over time. Also, the changes in the shapes of droplets are higher in the droplets at the rear wall compared to those at the center of the 2-dimensional channel. Shan and Chen [23] offered the possibility of interpreting the flow of different fluids that do not mix under the same temperature conditions using a lattice Boltzmann method. They offered the possibility of applying the method to various multi-phase flow problems. Swift et al. [24] introduced a free energy approach using a lattice Boltzmann method for the first time. Gunstensen et al. [25] proposed a non-mixing model of a flow surface. Wu et al. [26] proposed models that modified the pressure disturbance on the fluid surface based on the study results from Gunstensen at al. [25].

The present study uses the lattice Boltzmann method to examine the static behavior and dynamic behavior of the meniscus formed between an AFM tip and a solid substrate in a 3-dimensional channel. Studies on the dynamic behavior of the meniscus were performed for when the bottom wall moves with a constant velocity with a meniscus between the bottom wall and the flat tip. In order to find out the dynamic behavior of the meniscus, study considers the initial contact angles of the meniscus, the bottom wall, and the flat tip, as well as the moving velocity of the bottom wall.

2. Numerical methodology

2.1. Lattice Boltzmann method

The lattice Boltzmann method was used to simulate the static and dynamic behaviors of the meniscus between a bottom wall and a tip. The lattice Boltzmann equation was created by combining lattice-gas-automata (LGA) with the Boltzmann equation in order to overcome the weaknesses of Boolean algebra operation and the many models for flow simulations of fluids that have been developed so far and are being widely used in many fields.

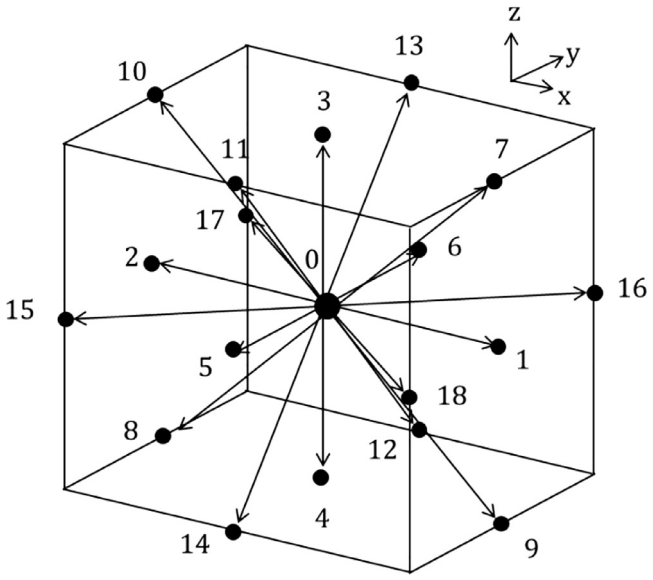

Fig. 1. D3Q19 lattice velocity vector directions used in the current model.

The discrete Boltzmann equation for transporting non-compressive discrete fluid particles can be represented as follows:

$$\frac{\partial f^k}{\partial t} + \mathbf{e} \cdot \nabla f^k = \Omega^k \tag{1}$$

where f^k, k, $\mathbf{e}$ and Ω^k represent the density distribution function of the fluid, the phase of each fluid, the particle velocity vector (lattice velocity vector), and the collision operator, respectively. The collision operator Ω^k is represented by Eq. (2) based on the assumption of BGK:

$$\Omega^k = -\frac{1}{\tau^k}(f - f^{eq}) \tag{2}$$

where τ^k and f_i^{eq} represent the single relaxation time and the equilibrium density distribution function for the kth fluid, respectively. The single relaxation time means the time for a system in equilibrium to return to the equilibrium state again after applying external forces. Thus, the Boltzmann equation can be expressed as Eq. (3).

$$\frac{\partial f^k}{\partial t} + \mathbf{e} \cdot \nabla f^k = -\frac{1}{\tau^k}\left(f - f^{(eq)}\right) \tag{3}$$

There is a unique equilibrium density distribution function according to the lattice model. This study uses the D3Q19 model with 19 velocities in a 3-dimensional space, as shown in Fig. 1. In this case, the following equilibrium density distribution function is used:

$$f_i^{k(eq)} = \omega_i \rho^k \left[1 + \frac{3}{c^2}(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2c^4}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2c^2}\mathbf{u} \cdot \mathbf{u}\right] \tag{4}$$

where ω_i, ρ, and $\mathbf{u}$ represent the weighting factor, fluid density, and fluid velocity vector, respectively. The weighting factor is analytically determined according to the type of the lattice and the direction and the size of the velocity in the lattice. The weighting factor is given as Eq. (5) in the D3Q19 model:

$$\omega_i = \begin{cases} 1/3 & i = 0 \\ 1/18 & i = 1, \cdots, 6 \\ 1/36 & i = 7, \cdots, 18 \end{cases} \tag{5}$$