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A numerical study on the dynamic behavior of the liquid droplet located on heterogeneous surface

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ABSTRACT

The behavior of a droplet located on a heterogeneous surface is numerically analyzed using the 3-D Lattice Boltzmann Method. Predictions are made whether the droplet will be separated or not and the separation time is calculated changing the contact angles of the hydrophilic surface, hydrophobic surface and the area of the hydrophobic surface. The change in the contacting length between the droplet and the bottom surface and the change in the dynamic contact angle of the droplet on the cross section at the center of the droplet as time passes are observed, and the droplet separation mechanism is investigated by analyzing the velocity vector around the phase boundary line and the droplet which changes with time while the shape of the droplet changes. A droplet located at the center of a heterogeneous surface shows a trend of being easily separated if the difference between the contact angles of the hydrophilic and hydrophobic surfaces is bigger. The more the contact angle of the hydrophilic surface increases, the more the droplet separation time increases, and the more the contact angle of the hydrophobic surface increases, the more the droplet separation time decreases. Also, though the droplet separation time shows a decreasing trend when the width of the hydrophobic surface increases, it does not have any effect on whether the droplet will be separated or not.

1. Introduction

Multiphase flow is an issue which attracts people's attention in diverse fields such as engineering, industry and environment as well as natural science including chemistry and biology. Being an important part in various fields from natural phenomena such as rainstorm, smog and snowstorm to industrial fields such as air conditioning system, refrigerating system, sea water desalination plant, nuclear power generation equipment, and various heat exchangers, it has attracted attention of many researchers. Studies on behaviors of droplets among multiphase flow issues are actively conducted experimentally or numerically with recent development of micro/nanotechnology. Tervino et al. [1], Yang and Koplik [2], and Gu and Li [3] conducted numerical studies on the phenomenon of a droplet spreading over a solid surface in a stationary state. Also, Bayer and Megaridis [4], Cossali et al. [5], Mao et al. [6], Sikalo et al. [7], and Zhang and Basaran [8] experimentally studied the behavior of a droplet crashing onto a solid surface. And Fujimoto et al. [9], and Manservisi and Scardovelli [10] conducted numerical studies on the dynamic behavior of a droplet colliding with a solid surface. Tanaka et al. [11] and Lunkad et al. [12] conducted numerical studies on the kinetic characteristics of a droplet moving on a slanted solid surface or on a solid surface to which a force was applied, and compared the result of the numerical analyses with the experimental result of Sikalo et al. [13].

Boltzmann Method (LBM) is a computational analysis technique which recently attracts people's attention by reason of its fast computation speed, multiphase analysis, and easiness of parallelization. Many studies have been conducted using the Lattice Boltzmann Method, and Shan and Chen [14] in particular presented a model capable of analyzing the multiphase flow of different fluids which do not mix with each other at the same temperature using the Lattice Boltzmann Method. Swift et al. [15] introduced a free energy approach into the multiphase flow model, and Gunstensen et al. [16] proposed a method of analyzing a two-phase flow using a multiple density distribution function. Wu et al. [17] presented a model of which the pressure disturbance was corrected at the phase boundary based on the research findings of Gunstensen et al. [16].

In this study, the behavior of a hemispherical droplet located on a heterogeneous surface was studied using the 3D Lattice Boltzmann Method. A hydrophobic bottom surface exists at the

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center of a hydrophilic bottom surface, and a hemispherical droplet is located at the center of the bottom surface lying from the hydrophilic bottom surface to the hydrophobic bottom surface. The droplet is separated or reaches a new equilibrium state without being separated depending on the contact angles of the hydrophilic and hydrophobic bottom surfaces. The time at which the droplet is separated differs depending on the width of the hydrophobic bottom surface, which also has an effect on whether or not the droplet will be separated. In this study, an investigation was carried out as to whether the droplet is separated or not changing the contact angle of the heterogeneous surfaces with different hydrophobic widths, and the change in the contacting length between the bottom surface and the droplet was presented. In the case the droplet was separated, the separation time of the droplet depending on the hydrophobic width and the contact angle of the bottom surface was calculated, and the dynamic contact angle between the bottom surface and the droplet which changes with time while the droplet is separated was calculated.

2. Numerical analysis method

2.1. Lattice Boltzmann Method

In this study, a 3D analysis was conducted on a droplet located on a heterogeneous surface using the Lattice Boltzmann Method. The governing equation was induced from the Boltzmann equation, and the application scope of the existing Lattice Gas Automata (LGA) governing equation was widened and its numerical stability was improved by expanding it to the real number range.

The discretized Boltzmann Equation for transportation of incompressible two-phase fluid particles is as follows:

$$\frac{\partial f_i^k}{\partial t} + \mathbf{e}_i \cdot \nabla f_i^k = \Omega_i^k \quad (1)$$

Here, f_i^k represents the density distribution function of the fluid particle, and the superscript k means the relevant phase. $\mathbf{e}_i$ means the lattice speed, and Ω_i^k means the collision operator. The subscript i represents the direction of the lattice, which is differently defined in accordance with the lattice model. Though the collision operator contains a very complicated mathematical mechanism, it can be simply expressed using the single relaxation time proposed by Bhatnahar et al. [18].

The discretized Boltzmann equation can be expressed as follows when simplified applying the BGK model [18]:

$$\frac{\partial f_i^k}{\partial t} + \mathbf{e}_i \cdot \nabla f_i^k = -\frac{1}{\tau^k}(f_i^k - f_i^{k(eq)}) \quad (2)$$

Here, τ^k represents the single relaxation time for the kth fluid, and $f_i^{k(eq)}$ represents the equilibrium distribution function. The equilibrium distribution function represents the value of the equilibrium state f_i^k has in the relaxation time.

The D3Q19 is a model considered for the fluid particle which can have a velocity in only 19 directions in a 3D space as shown in Fig. 1, and the lattice speed $\mathbf{e}_i$ is given as follows:

$$\begin{aligned} &\mathbf{e}_0 = (0,0,0) \\ &\mathbf{e}_{1,2}, \mathbf{e}_{3,4}, \mathbf{e}_{5,6} = (\pm1,0,0)c, (0,\pm1,0)c, (0,0,\pm1)c \\ &\mathbf{e}_{7,\ldots,10}, \mathbf{e}_{11,\ldots,14}, \mathbf{e}_{15,\ldots,18} = (\pm1,\pm1,0)c, (\pm1,0,\pm1)c, (0,\pm1,\pm1)c \end{aligned} \quad (3)$$

At this time, c is defined to be $\delta x/\delta t (c = \delta x/\delta t)$, and δx and δt represent the increments of space and time respectively. The Lattice Boltzmann Equation can be obtained by discretizing Eq. (2) for the unit time and lattice space which fall under lattice speed c.

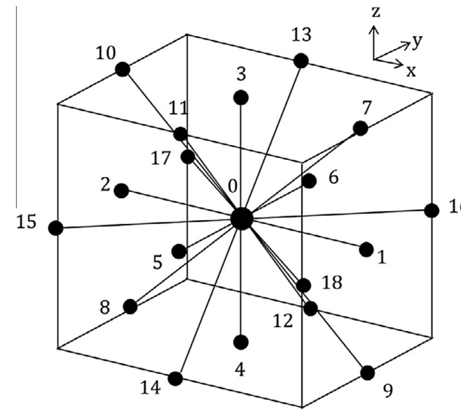

Fig. 1. The D3Q19 lattice model.

Accordingly, the Lattice Boltzmann Equation can be expressed as Eq. (4) below:

$$f_i^k(\mathbf{x}+\mathbf{e}_i, t+\delta t) - f_i^k(\mathbf{x},t) = -\frac{1}{\tau^k}(f_i^k - f_i^{k(eq)})_{(\mathbf{x},t)} \quad (4)$$

Here, the equilibrium distribution function $f_i^{k(eq)}$ is given as follows:

$$f_i^{k(eq)} = \omega_i \rho^k \left[1 + \frac{3}{c^2}(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2c^4}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2c^2}\mathbf{u}\cdot\mathbf{u}\right] \quad (5)$$

Here, ω_i is a weighting coefficient, and $\mathbf{u}$ represents the fluid velocity. In the model D3Q19, the weighting coefficient is given being divided into $\omega_0 = 1/3$, $\omega_i = 1/18$ $(i = 1, 2, 3, 4, 5, 6)$, and $\omega_i = 1/36$ $(i = 7, \ldots, 18)$ in accordance with the direction of the lattice speed. Eq. (4) used for the Lattice Boltzmann Method is alternately calculated being divided into the collision stage and flow stage, and has an advantage that, having a form of an explicit equation, the calculation speed is faster than the analysis which uses the Navier–Stokes equation discretized in the form of an implicit equation and calculations can be done in a microscopic area. Also, as the continuity equation and Navier–Stokes equation that govern flow of fluid can be induced from the BGK model based Lattice Boltzmann Method using the Chapman-Enskog theory, it can be confirmed that the Lattice Boltzmann Method can be also applied to macroscopic flow.

The macroscopic flow variables such as density (ρ) and pressure (p) are defined as follows:

$$\rho^k = \sum_i f_i^k = \sum_i f_i^{k(eq)} \quad (6)$$

$$\rho = \sum_k \rho^k \quad (7)$$

$$\rho\mathbf{u} = \sum_i f_i \mathbf{e}_i = \sum_i f_i^{eq}\mathbf{e}_i \quad (8)$$

$$p = \frac{1}{3}\rho c^2 \quad (9)$$

Here, ρ^k represents the fluid density of each phase.

2.2. Two-phase flow model

The two-phase model used in this study is the model proposed by Gunstensen et al. [16] and modified by Wu et al. [17]. This two-phase flow model is suitable to solve two-phase flows which do not mix with other fluids based on the lattice BGK model, and has a feature that there is no pressure disturbance at the phase boundary.

In the case two phases exist, the CSF (Continuum Surface Force) model was used to apply the surface tension at the boundary