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Research paper

Lattice Boltzmann parallel simulation of microflow dynamics over structured surfaces

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A B S T R A C T

In the present work, a parallel lattice Boltzmann multiphase model was developed to investigate the effects of surface structures on wettabilities and flow dynamics in a microchannel. The theory of wetting transition was firstly discussed. Then three types including triangular, rectangle and hierarchical shaped microstructures were constructed on the surface to examine the effects on wettabilities and drag reduction. It was found that flow behaviour is strongly affected by the surface morphology of the channel. The results indicated that hierarchical structures on the surface could improve the hydrophobicity significantly. For rectangular structures, they can improve the hydrophobicity with the increase of height and distance ratio h/d of the structures, and the improvement will reach its optimal hydrophobicity when the value h/d is over a certain value of 0.6. Moreover, to accelerate computational speed, the Open Multi-Processing (OpenMP) was employed for the parallelization of the model. A maximum speedup of 2.95 times was obtained for 4 threads on a multi-core CPU platform.

1. Introduction

Superhydrophobic surfaces with apparent water contact angles higher than 150° and low hysteresis have received immense interest in both scientific research and industrial field over the past decade, such as self-cleaning, anti-corrosion, drag reduction, drug delivery, optical devices, microfluidic devices and so forth [1]. These surfaces with high contact angle and low contact angle hysteresis with a self-cleaning effect also exhibit low adhesion and drag reduction for fluid flow [2]. Although superhydrophobic surfaces are usually designed with low surface free energy materials, the method of chemical surface modification alone can typically lead to water contact angles of up to 120° To achieve extreme values of contact angles larger than 150° (near 180°), the modification on surface structure has to be utilized [3]. The effects of surface roughness on wettability have been studied for a few decades after pioneering work carried out by Wenzel [4] and Cassie–Baxter [5] who proposed theoretical models to predict the wetting behaviour of the droplet in the non-composite and composite states. The superhydrophobicity mechanism of the lotus leaf was theoretically analysed by Marmur [6]. It has been found that the meta-stable states in the heterogeneous wetting regime play a key role in superhydrophobicity. A review paper regarding the impacts of surface roughness on wettabilities can be found in Ref. [7]. In order to construct artificial superhydrophobic surfaces, various methods and techniques have recently been developed. With these techniques, a great number of different surface morphologies have been fabricated successfully, such as the pillar morphology [8], flowerlike structure [9], ratchet-like morphology [10], the trapezoid morphology [11], and so on. Meanwhile, numerical studies have also been carried out extensively. Gao et al. [12] proposed a model to combine both factors caused by surface structure and energy change. They claimed that the Cassie–Baxter equation should be adopted for hierarchical roughness surface. Ambrosia et al. [13] used molecular dynamics simulations to investigate the hydrophobic properties of water droplets on regular pillared surface. It should be noted their work was limited to very small length and time scale due to the expensive computational cost of molecular dynamics method. A lattice Boltzmann model was developed to study the contact angles of droplets on the surfaces with regular roughness structures [14]. Lee et al. [15] has recently developed a lattice Boltzmann model to investigate the movement of droplet on stripe-patterned surfaces. Jung et al. [16] also employed the lattice Boltzmann method to determine the optimal geometry of microstructures to achieve superhydrophobicity. Their simulation results were also compared with the results of measured wettability of fabricated micro-hierarchical metal surface. However, the previous studies mainly focused on the effect of surface structures on

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Nomenclature

c	lattice speed
c_i	discrete particle speeds
c_s	speed of sound
f_i	density distribution function
feq	equilibrium distribution function
F_i	forcing term
g	gravitational acceleration
g_i	energy distribution function
k	effective thermal conductivity
w_i	weighting factor
G	fluid-fluid interaction strength
G_t	fluid-solid interaction strength

Greek Symbols

τ	relaxation time
ρ	density
μ	dynamic viscosity
ν	kinetic viscosity
Ω	collision operator
θ	contact angle

wettability and there are still few studies focusing on effects of the surface topography on drag reduction.

Over the past few years, the lattice Boltzmann method (LBM), a mesoscopic approach, has experienced tremendous advances and has been well accepted as a useful method to simulate various complex fluid phenomena, such as multiphase /multicomponent flows [17–19], electro-osmotic flow [20], micro/nano fluidics [21,22], Magneto-hydrodynamic flows [23,24], flows through porous media [25,26], reaction-diffusion system [27,28], and etc. Due to its kinetic nature and local dynamics, lattice Boltzmann method has several advantages over traditional numerical methods, including the physical representation of microscopic interactions, the easiness in dealing with complex geometries and parallelization of the algorithm. Recently, parallelization has become an important feature for numerical methods as high performance computing (HPC) are currently being designed for solving large-scale and complex engineering problems. The widely used parallel algorithms for LBM include multi-core CPUs [29], General Purpose GPU (GPGPU) [30] and hybrid CPU-GPU [31].

Based on our previous work on fabricating superhydrophobic surfaces and lattice Boltzmann simulating of complex fluids [22,23,32,33], we extended our research to numerical investigating of structured surfaces. The objective of this study is to develop a parallel LBM model to investigate the effects of different surface topography on the wettabilities and drag reduction. The rest of this paper is organized as follows: Section 2 introduces the methodology, including the multiphase lattice Boltzmann method, the wetting transition theory and the parallel algorithm. The performance of the parallelization and simulation results on wettabilities and drag reduction are given in Section 3. Finally, the conclusions are drawn in Section 4.

2. Methodology

2.1. The multiphase lattice Boltzmann method

The pseudo-potential lattice Boltzmann model for multicomponent multiphase fluid was employed in the present study [34]. The particle distribution function (PDF) of each component of the multiphase fluid satisfies the following equation:

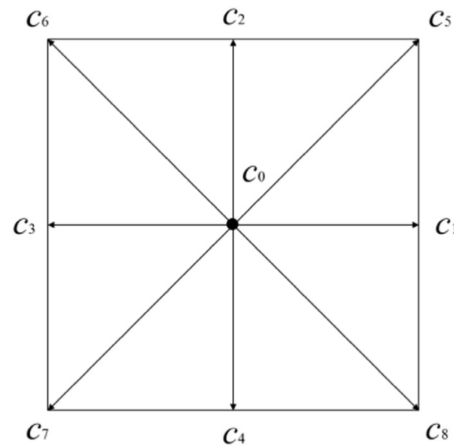

Fig. 1. Typical two dimensional lattice Boltzmann model (D2Q9).

$$f_i^\sigma(x + c_i\Delta t, t + \Delta t) - f_i^\sigma(x, t) = \Omega_{coll}^\sigma \tag{1}$$

where $f_i^\sigma(x,t)$ is the density distribution function of component σ and Ω_{coll}^σ is the collision operator, which has the form in the single-relaxation-time (SRT) LBM model:

$$\Omega_{coll}^\sigma = -\frac{1}{\tau^\sigma}\left(f_i^\sigma(x,t) - f_i^{\sigma,eq}(x,t)\right) \tag{2}$$

where τ^σ is a relaxation time which is related to its kinematic viscosity as $\nu^\sigma = c_s^2(\tau^\sigma - 0.5\Delta t)$. The equilibrium distribution function $f_i^{\sigma,eq}(x,t)$ can be calculated by the following equation:

$$f_i^{\sigma,eq} = \rho_\sigma w_i\left[1 + \frac{c_i\cdot u_\sigma^{eq}}{c_s^2} + \frac{(c_i\cdot u_\sigma^{eq})^2}{2c_s^4} - \frac{u_\sigma^{eq}\cdot u_\sigma^{eq}}{2c_s^2}\right] \tag{3}$$

where w_i are weighting factors specific to the chosen lattice. For the two-dimensional nine-velocity lattice Boltzmann model (D2Q9, as seen in Fig. 1) employed in this work, w_i are 4/9, 1/9 and 1/36, for $i = 0$, 1-–4, 5-–8, respectively [35]. ρ_σ is the density of component σ. c_s is the sound speed. c_i is the discrete velocities which are defined as:

$$c_i = \begin{cases} (0,0), i = 0 \\ c(\cos\theta_i, \sin\theta_i), (\theta_i = (i-1)\pi/2, i = 1,2,3,4) \\ \sqrt{2}c(\cos\theta_i, \sin\theta_i), (\theta_i = (i-5)\pi/2 + \pi/4, i = 5,6,7,8) \end{cases} \tag{4}$$

where c_i is the particle streaming speed and determined by $c = \Delta x/\Delta t$. Δx, Δt are the lattice spacing and time step, respectively. The relation between c_s and c can be expressed as $c_s = c/\sqrt{3}$. The macroscopic density and momentum of the σ th component are defined as:

$$\rho_\sigma = \sum_i f_i^\sigma \tag{5}$$

$$\rho_\sigma u_\sigma = \sum_i f_i^\sigma c_i \tag{6}$$

The equilibrium velocity u_σ^{eq} in Eq. (3) is defined as:

$$\rho_\sigma u_\sigma^{eq} = \rho_\sigma u' + \tau_\sigma F_\sigma \tag{7}$$

where u' is an effective velocity and $F_\sigma = F_{c,\sigma} + F_{ads,\sigma} + F_{e,\sigma}$ is the total force acting on the σth component including fluid-fluid interaction $F_{c,\sigma}$, fluid-solid interaction $F_{ads,\sigma}$ and external force $F_{e,\sigma}$. To conserve momentum in the absence of forces, u' should satisfy:

$$u' = \sum_\sigma \frac{\rho_\sigma u_\sigma}{\tau_\sigma} \Big/ \sum_\sigma \frac{\rho_\sigma}{\tau_\sigma} \tag{8}$$