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A Mass Conservative Lattice Boltzmann Model for Two-Phase Flows with Moving Contact Lines at High Density Ratio

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Abstract. In this paper, a mass conservative lattice Boltzmann model (LBM) is proposed to simulate the two-phase flows with moving contact lines at high density ratio. The proposed model consists of a phase field lattice Boltzmann equation (LBE) for solving the conservative Allen-Cahn (A-C) equation, and a pressure evolution LBE for solving the incompressible Navier-Stokes equations. In addition, a modified wall boundary treatment scheme is developed to ensure the mass conservation. The wetting dynamics are treated by incorporating the cubic wall energy in the expression of the total free energy. The current model is characterized by mass conservation, proper treatment of wetting boundary and high density ratio. We applied the model on a series of numerical tests including equilibrium droplets on wetting surfaces, co-current flow and a droplet moving by gravity along inclined wetting surfaces. Theoretical analysis and experiments were conducted for model validation. The numerical results show good performances on mass conservation even with a density contrast up to 1000. Furthermore, the results show that the moving contact line can be successfully recovered, which proves that this model is applicable on the study of moving contact line issue and further related applications.

AMS subject classifications: 76T10, 76M28, 76D99

Key words: Lattice Boltzmann model, two-phase flow, moving contact line, high density ratio.

1 Introduction

The behavior of droplets on wetting surfaces is always a popular research topic because it is the multiphase flow fundamental of many engineering applications. The contact

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angle, which is defined as the angle between the contact line and the solid surface, is an important parameter characterizing the wettability, which significantly influences the behavior of droplets on wetting surfaces. If the solid surface is not horizontal and the gravity exists, the droplet may move on the surface and so as the triple contact line. In this situation, the moving contact line is observed and dynamic contact angles should be defined to feature this phenomenon. The study of the moving contact line is of great significance in engineering applications such like chip cooling, painting, coating and falling film based liquid desiccant technology [1,2]. The mechanism of formation of contact line has been studied theoretically by many researchers [3,4] and it is possible to predict the final equilibrium state of contact lines. However, the transition process, which is important for understanding the mechanism of moving contact line phenomenon, has not been sufficiently understood in previous theoretical studies. Considering the difficulties in conducting experimental study, numerical methods are more competent for studying the moving contact line.

The lattice Boltzmann method (LBM), which is a numerical method rooted in kinetic theory, is becoming popular in the fields of computational fluid dynamics in last decades [5]. Due to the particle-based mesoscopic nature which connects the micro and macro worlds, the LBM has an advantage in simulation fidelity and computational efficiency especially for some complicated flows such as turbulent flows [6, 7] and multiphase flows [8, 9]. A number of LB models for multiphase flows have been developed in previous researches [10], such as color-gradient model [11], Shan-Chen model [12, 13], free energy model [14, 15] and phase-field model [16, 17]. An extended Shan-Chen method, in which the equation of state (EOS) and surface tension can be tuned independently, was developed by Sbragaglia et al. [18] to analyze the physical behavior of a class of mesoscopic models for multiphase flows. Colosqui et al. [19] presented a dynamic optimization strategy to generate customized equations of state for the numerical simulation of non-ideal fluids at high density ratio. The phase-field LB model, which is originally developed by He et al. [16] in 1998, has been proved applicable to high density ratio issue, which is a key challenge in modelling moving contact angle. Two distribution functions are taken in this model, one is for describing the fluid dynamics and the other is used to track the phase interface, and two macroscopic equations can be recovered from the distribution functions. The combination of Navier-Stokes (N-S) and Cahn-Hilliard (C-H) equation is applied in many phase field LBMs. Lee and Liu [20] successfully simulate the contact angle at high density ratio with a proposed C-H based LBM. Liang et al. [21] reported their C-H based LBM can properly describe the axisymmetric multiphase flows. However, due to the simplification made in the recovering process, the C-H based phase field LBMs cannot ensure mass conservation. Around 1% of mass change ratio was observed in Connington and Lee's work [22]. Although the error is not large, it may be unacceptable in some special applications. For example, Zheng et al. [23] reported that in their modelling, the small droplet disappeared if the radius was below a critical value. A conservative LBM for interface tracking was proposed by Fakhari et al. [24] in 2016. The model was also based on the phase field theory, but it recovered the Allen-Cahn (A-C)