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Lattice Boltzmann Simulation of Particle Motion in Binary Immiscible Fluids

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Abstract. We combine the Shan-Chen multicomponent lattice Boltzmann model and the link-based bounce-back particle suspension model to simulate particle motion in binary immiscible fluids. The impact of the slightly mixing nature of the Shan-Chen model and the fluid density variations near the solid surface caused by the fluid-solid interaction, on the particle motion in binary fluids is comprehensively studied. Our simulations show that existing models suffer significant fluid mass drift as the particle moves across nodes, and the obtained particle trajectories deviate away from the correct ones. A modified wetting model is then proposed to reduce the non-physical effects, and its effectiveness is validated by comparison with existing wetting models. Furthermore, the first-order refill method for the newly created lattice node combined with the new wetting model significantly improves mass conservation and accuracy.

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Key words: Lattice Boltzmann model, particle suspension model, binary immiscible fluids.

1 Introduction

Particle suspension in multiphase or multicomponent flows has gained increasing attention during the last decade [3, 4, 16, 20, 23, 24, 28, 32, 41, 42], due to the extensive use

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of particles to stablize emulsions, which has many applications in food, cosmetics and medical industires [23], as well as the use of proppants in hydraulic fracturing for unconventional gas production [36]. Also, in many processes, such as hydrocarbon recovery, geologic CO_2 sequestration, and soil wetting and drying, understanding the emergent patterns of the invasion of one fluid into a deformable porous medium filled with another fluid is both scientifically fascinating and technologically important [21]. If the deformable porous medium is modeled by the discrete element method [14], then it all boils down to the problem of accurately simulating particle suspension in multiphase or multicomponent flow.

Numerical simulation of particle suspension in multiphase or multicomponent flows requires accurately capturing the motion of particle and the interface of the fluid, neither of which can be easily accomplished by traditional CFD method. The lattice Boltzmann method (LBM) has become a powerful numerical tool to model complex flow and multi-physicochemical transport processes [1,9,43,44], and is suitable to fulfill the above requirements, mainly due to the fact that it is based on microscopic models and mesoscopic kinetic equations [9]. It has already been employed to simulate particle suspension in multiphase or multicomponent flows [16,23,24,28,32,41,42]. The link-based lattice Boltzmann particle suspension model, first proposed by Ladd [26] and further developed by Aidun *et al.* [2], has been widely used and the LBM simulation results are comparable to the finite element results [11, 34]. For modeling multiphase or multicomponent flow, the Shan-Chen pseudo-potential lattice Boltzmann model [8, 33, 37–39] has been applied with considerable success [1]. In this paper, we combine the link-based particle suspension model and the classic Shan-Chen multicomponent model [38] to simulate particle suspension in binary immiscible fluids.

Previous LBM approaches have reported mass non-conservation issue [23, 41] when the fluid information inside the particle is excluded. Although retaining fluid information inside the particle can ensure exact mass conservation in the whole computation domain including the solid particle region [24, 28, 32], the fluid mass may not be conserved in the fluid region outside the particle. Also, when introducing non-neutral wetting, additional wetting forces will act on the solid particle, and nonphysical effects such as density variations near solid surface affect the motion of the particle. Simulation accuracy may be decreased compared with single phase flow simulations, which has not been well studied. Therefore, in this paper, we will focus on the accuracy and mass conservation of the existing approaches, and propose a modified approach to reduce mass non-conservation and to improve accuracy.

The rest of the paper is organized as follows. Section 2 introduces the numerical methods of this paper, including the Shan-Chen multicomponent model, particle suspension model and related modifications required in combining these two models. In Section 3, we perform extensive numerical simulations to validate our method and compare the results with existing methods. Section 4 concludes the paper.