

Investigating Droplet and Bubble Deformation under Shear Flow using the Multi-Pseudo-Potential Scheme of Lattice Boltzmann Method

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Abstract. In the present study, a multi-pseudo-potential model is used to simulate the deformation and breakup of bubbles and droplets under simple shear flow. It is shown that the current model can adjust the amount of surface tension, independent of the interface thickness, equation of state (EOS), and reduced temperature. Considering the available findings, no comprehensive study has been performed on all aspects of deformation of bubbles and droplets under shear flow using numerical methods. Bubble or droplet deformation under simple shear flow depends on two non-dimensional numbers: capillary number (Ca) and viscosity ratio (λ). In this investigation, various scenarios, including small deformation, large deformation, and breakup for bubbles ($0.2 < \lambda < 1$) and droplets ($1 < \lambda < 5$), are separately studied. Results of the multi-pseudo-potential model show that the bubble and droplet deformations oscillate under shear flow and undergo elongation and contraction over time to converge to the final shape. As the capillary increases by more than one, the bubble expands and shrinks. The bubble tips become sharp, and so-called slender, at a low viscosity ratio (λ). A detailed comparison is made between the numerical results for deformation parameters of the present model and the experimental results available in the references.

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Key words: Lattice Boltzmann method, multi-pseudo-potential scheme, droplet and bubble deformation, simple shear flow, capillary number.

1 Introduction

Multiphase flow is considered a continuum fluid flow with two different phases (i.e., gas and liquid) [1-3] and has particular importance in industrial and scientific applications [4]. Various numerical methods have been developed based on the macroscopic

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approach, all of which require tracking the interface between the two phases in the flow simulation. However, the methods based on the mesoscopic approach, such as lattice Boltzmann method (LBM), can automatically detect the border of each phase without any extra calculations [5-7]. Besides, these methods do not require using the Poisson's equation for pressure correction. These specifications of the mesoscopic models make it possible to model two-phase flows with a more straightforward implementation algorithm and less computational cost than those for the conventional computational fluid dynamic schemes [8-10].

Color-gradient [11], Shan-Chen [12, 13], and free-energy [14, 15] are the three categories that have been introduced so far for the multiphase LBMs. Observations show that the Shan-Chen category has attracted more attention, which is due to the ease of implementation and robust description of particle interactions [3]. The main concern in using the Shan-Chen model is to achieve full thermodynamic consistency [16-18], meaning that energy conservation is maintained in the phase transition [16].

In the original Shan-Chen method, the interaction force between the particles is modeled by a pseudo-potential function (ψ). Numerous investigations have been performed on the relationship between pseudo-potential function and density of phases on the thermodynamic consistency [2, 3, 17, 19]. He and Doolen's [20] results demonstrated that the pseudo-potential function must be defined according to the density ($\psi \propto \rho$) to achieve thermodynamic consistency. However, it is necessary to consider a suitable relationship between the pseudo-potential function and density in order to accurately calculate the pressure tensor [21]. Accordingly, Shan and Chen [13] demonstrated that $\psi = \psi_0 \exp -\rho_0/\rho$ could properly model pressure tensor. In another study, Sbragaglia et al. [22] showed that Shan's relation increased numerical instability and spurious velocities near the interface.

As mentioned earlier, the energy conservation must be satisfied in order to obtain a thermodynamically consistent model. Since the free energy method maintains this criterion, Sbragaglia and Shan tried to coincide the Shan-Chen model with the free energy method [23]. Their suggestion was to define a pseudo-potential function as $\psi = (\rho/(E+\rho))^{(1/E)}$, where E is a constant depending on the lattice [23, 24].

Various approaches have been taken to correct the shortcomings of the original Shan-Chen model, in all of which the idea of using a pseudo-potential function has been preserved. The results show this approach cannot take into account all the aspects related to intermolecular forces. Therefore, it cannot eliminate the thermodynamic inconsistency of the original Shan-Chen model [25, 26]. Accordingly, in the present study, a multi-pseudo-potential model is introduced to simulate two-phase flows. Each of the pseudo-potential functions is responsible for modeling a portion of the intermolecular forces. The suggestion of Sbragaglia and Shan has also been used to satisfy energy conservation. Khajepoor and Chen [17] represented that the multi-pseudo-potential scheme was utterly consistent with thermodynamics and could be used for engineering applications. Their results displayed this approach could reduce the spurious velocities in the interface of two phases. The multi-pseudo-potential Shan-Chen model can adjust the amount of surface tension,