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A Pseudopotential Lattice Boltzmann Analysis for Multicomponent Flow

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Abstract. This paper presents a pseudopotential lattice Boltzmann analysis to show the deficiency of previous pseudopotential models, i.e., inconsistency between equilibrium velocity and mixture velocity. To rectify this problem, there are two strategies: decoupling relaxation time and kinematic viscosity or introducing a system mixture relaxation time. Then, we constructed two modified models: a two-relaxation-time (TRT) scheme and a triple-relaxation-time (TriRT) scheme to decouple the relaxation time and kinematic viscosity. Meanwhile, inspired by the idea of a system mixture relaxation time, we developed three mixture models under different collision schemes, viz. mix-SRT, mix-TRT, and mix-TriRT models. Afterwards, we derived the advection-diffusion equation for the multicomponent system and derived the mutual diffusivity in a binary mixture. Finally, we conducted several numerical simulations to validate the analysis on these models. The numerical results show that these models can obtain smaller spurious currents than previous models and have a wider range for the accessible viscosity ratio with fourth-order isotropy. Compared to previous models, present models avoid complex matrix operations and only fourth-order isotropy is required. The increased simplicity and higher computational efficiency of these models make them easy to apply to engineering and industrial applications.

AMS subject classifications: 76M28, 76T06

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1 Introduction

During the past three decades, the pseudopotential lattice Boltzmann (LB) model has been widely employed in multicomponent flows owing to its simplicity and efficiency [1–7]. In the original pseudopotential model [8,9], an interparticle potential has been utilized to mimic the interaction between different phases or components, which in turn induce an interaction force to control the phase separation. As a consequence, the phase separation occurs automatically without tracking or capturing the interfaces between different phases. Such a simple approach does have some limits, namely large spurious currents in the vicinity of the phase interface [10], and numerical instability for high density/viscosity ratio [11].

In order to meet the demand for engineering, the LB community has been working on improving the accessible density/viscosity ratio while reducing the spurious currents. One major approach is to incorporate various equations of state (EOS) into the functional form of the interparticle potential. Yuan and Schaefer [12] found that the density ratio can be significantly enhanced by incorporating an appropriate equation of state through several numerical investigations for the single-component systems. Kupershtokh [13] proposed a linear combination of the local and mean value gradient approximations for evaluating the interaction force, which leads to obtaining a high-density ratio (up to 10^9 for the stationary case). Bao and Schaefer introduced an LB model that can simulate multicomponent systems with density ratios approaching 1000:1, which makes it possible to simulate and investigate the composition of gas and liquid. Hu et al. [14] introduced a single parameter in EOS that results in an easily achievable large density ratio. Other possible approaches are to use a higher-order isotropic gradient operator or modify the collision scheme of the LB model. In 2006, Shan [10] found that the spurious currents mainly arise from the insufficient isotropy of the discrete gradient operator and can be significantly reduced by adopting a higher-order isotropy gradient operator in calculating the interaction force. Later, Sbragaglia et al. [15] proposed a generalized LB model with multirange pseudopotential, and pointed out that when a higher-order isotropic gradient operator is adopted, the implementation of solid boundary conditions will become complex. Yu and Fan [16] showed that by adopting a multiple-relaxation-time (MRT) collision scheme, the spurious currents can be reduced as compared with single-relaxation-time (SRT) collision scheme. Moreover, Li et al. developed an improved forcing scheme based on the MRT collision scheme and found that the influence of viscosity at large density ratios can be significantly reduced by using the MRT collision model. Fei et al. [17] developed a three-dimensional MRT model based on a set of non-orthogonal basis vectors for the multiphase flow with a large density ratio. Compared with the classical MRT model [18], the non-orthogonal MRT model is simplified in implementation and has enhanced computational efficiency.

The numerical instability of multicomponent systems with large density ratios has almost been solved, but the research on multicomponent systems with large viscosity ratios is at its first stage. With the early pseudopotential LB model, the viscosity ra-