Journal of Computational Physics 327 (2016) 121–139

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

# Third-order analysis of pseudopotential lattice Boltzmann model for multiphase flow

Rongzong Huang, Huiying Wu *

*Key Laboratory for Power Machinery and Engineering of Ministry of Education, School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai 200240, China*

ARTICLE INFO

*Article history:*
Received 2 May 2016
Received in revised form 28 August 2016
Accepted 12 September 2016
Available online 16 September 2016

*Keywords:*
Pseudopotential lattice Boltzmann model
Third-order analysis
Multiple-relaxation-time
Isotropic property
Pressure tensor
Third-order additional term

ABSTRACT

In this work, a third-order Chapman–Enskog analysis of the multiple-relaxation-time (MRT) pseudopotential lattice Boltzmann (LB) model for multiphase flow is performed for the first time. The leading terms on the interaction force, consisting of an anisotropic and an isotropic term, are successfully identified in the third-order macroscopic equation recovered by the lattice Boltzmann equation (LBE), and then new mathematical insights into the pseudopotential LB model are provided. For the third-order anisotropic term, numerical tests show that it can cause the stationary droplet to become out-of-round, which suggests the isotropic property of the LBE needs to be seriously considered in the pseudopotential LB model. By adopting the classical equilibrium moment or setting the so-called "magic" parameter to 1/12, the anisotropic term can be eliminated, which is found from the present third-order analysis and also validated numerically. As for the third-order isotropic term, when and only when it is considered, accurate *continuum form* pressure tensor can be definitely obtained, by which the predicted coexistence densities always agree well with the numerical results. Compared with this *continuum form* pressure tensor, the classical *discrete form* pressure tensor is accurate only when the isotropic term is a specific one. At last, in the framework of the present third-order analysis, a consistent scheme for third-order additional term is proposed, which can be used to independently adjust the coexistence densities and surface tension. Numerical tests are subsequently carried out to validate the present scheme.



## 1. Introduction

Multiphase flows are widely encountered in lots of natural and engineering systems, such as falling raindrop, cloud formation, droplet-based microfluidic, phase-change device, etc. Due to the existence of the deformable phase interface whose position is unknown in advance, numerical simulation of multiphase flow is much more complicated than that of single-phase flow. As a powerful and attractive mesoscopic approach for simulating complex fluid flow problem, the lattice Boltzmann (LB) method has been applied to the simulation of multiphase flow in past years [1–4]. Generally, the existing LB methods for multiphase flow can be grouped into four major categories: (1) the color-gradient LB method [5–8], (2) the pseudopotential LB method [9–13], (3) the free-energy LB method [14–17], and (4) the kinetic-theory-based LB method [18–21]. Among these LB methods, the pseudopotential LB method, originally proposed by Shan and Chen [9,10],

* Corresponding author.
*E-mail address:* whysrj@sjtu.edu.cn (H. Wu).

http://dx.doi.org/10.1016/j.jcp.2016.09.030

is the simplest one in both concept and computation, and thus becomes particularly popular in the LB community for the simulation of multiphase flow.

In the pseudopotential LB model for multiphase flow, an interaction force is introduced to mimic the underlying intermolecular interactions, which are responsible for the formation of multiphase flow. Consequently, phase transition or separation can be automatically achieved, and thus the conventional interface capturing and tracking methods are avoided. Essentially speaking, the interaction force, which is incorporated into the lattice Boltzmann equation (LBE) through a general forcing scheme, can be viewed as a finite-difference gradient operator to recover the non-ideal gas component of the non-monotonic equation of state (EOS) [22] (i.e., $p_{\rm EOS} - p^{\rm ideal}$, where $p_{\rm EOS}$ and $p^{\rm ideal}$ denote the non-monotonic EOS and its ideal gas component, respectively). Simultaneously, the interfacial dynamics, such as the non-zero surface tension, are automatically produced by the higher-order terms in the finite-difference gradient operator. Due to such simple and integrated treatments of the interfacial dynamics, some well-known drawbacks exist in the pseudopotential LB model, though its application has been particularly fruitful [23–28].

One drawback of the pseudopotential LB model is the relatively large spurious current near the curved phase interface, especially at a large density ratio. Shan [22] argued that the spurious current is caused by the insufficient isotropy of the interaction force (as a finite-difference gradient operator), and inferred that the spurious current can be made arbitrarily small by increasing the degree of isotropy of the interaction force, which is realized by counting the interactions beyond nearest-neighbor. Numerical tests show the spurious current is suppressed to some extent by Shan's method [11,22], and counting more neighbors will complicate the boundary condition treatment. Sbragaglia et al. [11] investigated the refinement of phase interface and found that the spurious current can be remarkably reduced by widening the phase interface (in lattice units). Afterwards, some more methods were proposed to adjust the interface thickness [29–31]. Recently, Guo et al. [32] and Xiong and Guo [33] analyzed the force balance condition at the discrete lattice level of LBE, and found that the spurious current is partly caused by the intrinsic force imbalance in the LBE. Besides the above works, some other researches have also been made to shed light on the origin of the spurious current [34] and to provide way to reduce the spurious current [35].

Another two drawbacks of the pseudopotential LB model are the thermodynamic inconsistency (the coexistence densities are inconsistent with the thermodynamic results) and the nonadjustable surface tension (the surface tension cannot be adjusted independently of the coexistence densities). Both of these two drawbacks stem from the simple and integrated treatments of the interfacial dynamics, since the coexistence densities and surface tension are affected, or even determined, by the higher-order terms in the interaction force. In the pseudopotential LB community, it has been widely shown that different forcing schemes for incorporating the interaction force into LBE yield distinctly different coexistence densities (particularly the gas density at a large density ratio) [30,36–38]. Li et al. [12] found that the rationale behind this phenomenon is that different forcing schemes produce different additional terms in the recovered macroscopic equation, which have important influences on the interfacial dynamics for multiphase flow, and then they proposed a forcing scheme to alleviate the thermodynamic inconsistency. Following the similar way, some other forcing schemes have been proposed recently [31,39,40]. As compared to the thermodynamic inconsistency, the nonadjustable surface tension has not received much attention. In 2007, Sbragaglia et al. [11] first proposed a multirange pseudopotential LB model, where the surface tension can be adjusted independently of the EOS. However, as shown by Huang et al.'s numerical tests [30], the coexistence densities, which are not only determined by the EOS but also affected by the interfacial dynamics, still vary with the adjustment of the surface tension. By introducing a source term into LBE to incorporate specific additional term, Li and Luo [41] proposed a nearest-neighbor-based approach to adjust the surface tension independently of the coexistence densities. Similar additional term was also utilized to independently adjust the surface tension in the latter work by Lycett-Brown and Luo [40].

Up to date, the above drawbacks in the pseudopotential LB model have been widely investigated and the corresponding theoretical foundations for the pseudopotential LB model have been further consolidated. However, there still exist some theoretical aspects unclear or inconsistent in the pseudopotential LB model. The isotropic property of the LBE has not been investigated although this aspect of the interaction force has been clearly clarified. Accurate pressure tensor cannot be obtained from the recovered macroscopic equation and the reason is still unclear. Some additional terms, like $\nabla \cdot (h\mathbf{FF})$ ($h$ is a coefficient and $\mathbf{F}$ is the interaction force), should be recovered at the third-order through the Chapman–Enskog analysis, but such terms are inconsistently recovered at the second-order previously. To understand these unclear or inconsistent theoretical aspects, the traditional second-order Chapman–Enskog analysis, which is adopted in nearly all previous works, is insufficient, and higher-order analysis is required. In this work, we target on these theoretical aspects, and perform a third-order Chapman–Enskog analysis of the multiple-relaxation-time (MRT) pseudopotential LB model for multiphase flow. The remainder of the present paper is organized as follows. Section 2 briefly introduces the MRT pseudopotential LB model. Section 3 gives the standard second-order Chapman–Enskog analysis. In Section 4, a third-order Chapman–Enskog analysis of the MRT pseudopotential LB model is performed. In Section 5, the theoretical results of the third-order analysis are discussed detailedly and validated numerically. In Section 6, a consistent scheme for third-order additional term is proposed to independently adjust the coexistence densities and surface tension. At last, a brief conclusion is drawn in Section 7.

## 2. MRT pseudopotential LB model

Without loss of generality, a two-dimensional nine-velocity (D2Q9) MRT pseudopotential LB model is considered in this work. In the D2Q9 lattice, discrete velocities are given as