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Multiple-relaxation-time lattice Boltzmann model for binary mixtures of nonideal fluids based on the Enskog kinetic theory

Kang Yang · Zhaoli Guo

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Abstract In this paper, a lattice Boltzmann equation (LBE) model with multiple-relaxation-time (MRT) collision operator is developed based on the Enskog theory for isothermal nonideal mixtures, which is an extension of the previous single relaxation time (SRT) LBE model (Guo and Zhao in Phys Rev E 68:035302, 2003). The present MRT-LBE model overcomes some inherent defects of the original SRT-LBE model such as the fixed Schmidt number and limited viscosity ratio. It is also interestingly shown that the widely used Shan-Chen (SC) model, which is constructed heuristically based on the pseudo-potential concept, can also be regarded as a special case of the present model, and thus putting a solid foundation for this well-accepted multiphase LBE model. A series of numerical simulations, including the static droplet and layered co-current flow, are conducted to test the applicability of the present model for immiscible fluids with different Schmidt numbers and large viscosity ratio, which may be difficult for the original SRT-LBE model and the SC model.

Keywords Lattice Boltzmann equation · Enskog equation · Bhatnagar–Gross–Krook · Single relaxation time · Multiple-relaxation-time

1 Introduction

Numerical simulations of multiphase fluid flows play an important role in many engineering problems and natural processes. Traditional computational fluid dynamics (CFD) methods based on the Navier–Stokes equations, such as the volume of fluid [1] method and the level set method [2], are usually difficult to capture the interfacial dynamics due to the large disparity of temporal and spatial scales involved. The lattice Boltzmann equation (LBE) method [3], which is based on kinetic theory or micro particle dynamics, provides an alternative way for simulating multiphase flows by modeling the microscopic interaction among fluids. Actually, the LBE has found wide applications in the study of multiphase flows in the past decades, ranging from single-component to multicomponent fluids.

Several types of LBE models for multiphase flows have been developed from different viewpoints, such as the color models [4–6], pseudo-potential models [7–11], free energy models [12–14], phase-field models [15, 16], and kinetic theory-based models [17–22]. Among the above models, the pseudo-potential and free energy models have been extensively accepted and applied by physicists and engineers in the field of multiphase fluid flows, such as droplet/bubble dynamics [23–28], contact line movement [14, 29–33], phase separation [34–42], and multiphase flows in porous media [43–46]. The pseudo-potential models are popularly used due to their simplicity in the treatment of interparticle interactions. The basic idea is to mimic the microscopic molecular interaction at the mesoscopic scale using a pseudo-potential depending on a local density function. However, theoretical analysis shows that the pseudo-potential models are consistent with thermodynamic theories only when the local density function takes a special exponent form [8]. On the other hand, the

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K. Yang · Z. Guo (✉)
State Key Laboratory of Coal Combustion, Huazhong,
University of Science and Technology, Wuhan 430074, China
e-mail: zlguo@hust.edu.cn

free energy models, which are constructed based on free energy theory, do not suffer from this problem. A limitation of this model is the lack of Galilean invariance that is restored by several improved free energy models [27, 47, 48]. More recently, Xu et al. [40] proposed a new version of free energy LBE model which the reduced scalar pressure has a reasonable correlation to the density and sound speed, and the new model has been employed in a variety of studies [49, 50]. Besides the isothermal free energy models, thermal LBE models for multiphase system have also been developed, such as the model proposed in Ref. [51]. Gan et al. [52] further developed the model by employing the fast Fourier transform (FFT) so that the energy conservation is better satisfied and the spurious velocities can be damped to negligible scale. The improved model was successfully applied to the thermal liquid–vapor separation problem [53].

It should be noted that although the pseudo-potential and free energy models have been widely used, they are in lack of solid theoretical foundation which maybe leads to some drawbacks [18]. Subsequently, the LBE models based on certain kinetic models for nonideal fluids are proposed. For instance, Guo and Zhao [21, 22] developed two LBE models for dense binary fluids under isothermal conditions based on the Enskog equation. However, due to the use of single relaxation time (SRT) or Bhatnagar–Gross–Krook (BGK) collision operator, some inherent defects exist in both LBE models, such as the limited viscosity ratio and the fixed Schmidt number. These defects severely limit the applications of these models.

In order to overcome the above limitations and retain the clear physics picture of kinetic theory in LBE model, in this work we will propose an improved isothermal model for dense binary fluids with a multiple-relaxation-time (MRT) collision operator [54, 55] based on the Enskog kinetic theory. With the use of different relaxation times for different modes, the numerical stability of the LBE can be much improved and the applicable viscosity ratio range can be enlarged significantly. Furthermore, the viscosity and diffusivity can be determined from different relaxation times so that the Schmidt can be adjusted freely.

2 Simplified Enskog model for nonideal binary mixtures

Our starting point is the Enskog equation for a nonideal binary mixture [56, 57]

$$(D_a + \boldsymbol{g}_a \cdot \boldsymbol{\nabla}_{\boldsymbol{v}_a}) f_a(\boldsymbol{x}, \boldsymbol{v}_a, t) = J_{aa} + J_{ab}, \tag{1}$$

where the subscript a denotes the component (0 or 1) and b is the opposite to a, $D_a = \partial_t + \boldsymbol{v}_a \cdot \boldsymbol{\nabla}$ is the streaming operator, and $f_a(\boldsymbol{x}, \boldsymbol{v}_a, t)$ is the single-particle distribution function for component a at position $\boldsymbol{x}$ with velocity $\boldsymbol{v}_a$ at time t, $\boldsymbol{g}_a$ is the acceleration due to an external force acting on the particle of component a. J_{ac} is the collision operator between the particles of component a and c $(= a, b)$ and is given by

$$\begin{aligned} J_{ac} = \int \mathrm{d}\mu_{ac} [&\chi_{ac}(\boldsymbol{x} + y_{ac}\boldsymbol{k}) f_c(\boldsymbol{x} + \sigma_{ac}\boldsymbol{k}, \boldsymbol{v}_c') f_a(\boldsymbol{x}, \boldsymbol{v}_a') - \\ &\chi_{ac}(\boldsymbol{x} - y_{ac}\boldsymbol{k}) f_c(\boldsymbol{x} - \sigma_{ac}\boldsymbol{k}, \boldsymbol{v}_c) f_a(\boldsymbol{x}, \boldsymbol{v}_a)], \end{aligned} \tag{2}$$

where χ_{ac} is the radial distribution function (RDF), $y_{ac} = \sigma_{ac}/2$ with $\sigma_{ac} = (\sigma_a + \sigma_c)/2$, σ_i is the molecular diameter of species i; $\boldsymbol{k}$ is the unit vector directed from molecule c to particle a along the line of centers of the two colliding particles, $\boldsymbol{v}$ and $\boldsymbol{v}'$ are the molecular velocities before and after the collision, respectively. The number density for component a and the mixture velocity are defined as

$$n_a = \int f_a \mathrm{d}\boldsymbol{v}_a, \quad \rho \boldsymbol{u} = \sum_a m_a \int \boldsymbol{v}_a f_a \mathrm{d}\boldsymbol{v}_a, \tag{3}$$

where m_a is the particle mass for component a and $\rho = \sum_a m_a n_a$ is the density of the mixture.

The collision operator in the Enskog model is complicated and is difficult for devising numerical methods. A simplified Enskog model was developed for isothermal systems [22] based on Eq. (1),

$$D_a f_a(\boldsymbol{x} + \boldsymbol{v}_a, t) = -\frac{1}{\lambda}\left[f_a - f_a^{(\mathrm{eq})}\right] + \bar{\boldsymbol{F}}_a, \tag{4}$$

where $\bar{\boldsymbol{F}}_a$ is the total force including the inter-particle and external forces,

$$\bar{\boldsymbol{F}}_a = \frac{(\boldsymbol{v}_a - \boldsymbol{u}) \cdot \boldsymbol{F}_a}{\rho_a \theta_a} f_a^{(\mathrm{eq})}, \tag{5}$$

$$\boldsymbol{F}_a = \boldsymbol{F}_{\mathrm{ap}} + \boldsymbol{F}_{\mathrm{ae}} = -\rho_a \boldsymbol{K}_a \theta_a + \rho_a \boldsymbol{g}_a, \tag{6}$$

with $\boldsymbol{K}_a = \sum_c b_{ac} \rho_c \chi_{ac} \nabla \ln(\rho_c^2 \chi_{ac})$, and $b_{ac} = V_{ac}/m_c$ the second virial coefficient, $V_{ac} = 2^{D-1} V_D \sigma_{ac}^D$, and $V_D = (\pi/4)^{D/2}/\Gamma(1 + D/2)$ (Γ is the Gamma function). $f_a^{(\mathrm{eq})}$ is the local equilibrium distribution function given by

$$f_a^{(\mathrm{eq})} = n_a (2\pi\theta_a)^{-D/2} \exp[-(\boldsymbol{v}_a - \boldsymbol{u})^2/(2\theta_a)], \tag{7}$$

where $\theta_a = k_{\mathrm{B}} T/m_a$ is the normalized temperature with temperature T and Boltzmann constant k_{B}, $\boldsymbol{u}$ is the local barycentric velocity of the mixture, and λ is the relaxation time.

The model (4) is for nonideal gases. In the presence of interfaces between the two components, an additional surface force should be included, which can be written as

$$\boldsymbol{F}_{as} = \kappa n_a \boldsymbol{\nabla} \nabla^2 n_a, \tag{8}$$

where the parameter κ is related to the strength of surface tension.