Entropic Lattice Boltzmann Method for Simulation of Binary Mixtures

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Abstract

A new kinetic model for binary mixtures and its Lattice Boltzman (LB) discretization is presented. In the hydrodynamic limit the model recovers the Navier-Stokes and the Stefan-Maxwell binary diffusion equations. The thermodynamic consistency is ensured by the defined non-negative entropy production within the domain of applicability of the model. The present formulation is able to simulate mixtures with different Schmidt numbers and with a large molecular weight ratio of the components.

Key words: Lattice Boltzmann, BGK, Binary Mixtures

1 Introduction

Traditionally, the mass and momentum transfer in engineering flows is modeled using the continuum approach. However, in applications such as porous media, where sizes can be comparable to the mean free path of the gases, the use of kinetic theory is required. Recent success of kinetic algorithms such as the lattice Boltzmann method (Higuera *et al.* (1989); Qian *et al.* (1992);

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Ansumali *et al.* (2003)) showed that use of the kinetic theory approach might be benifical in the continuum domain too. Thus, it seems natural to extend the lattice Boltzmann approach to mixtures. Indeed, recently some LB models were proposed for mixtures (for recent a review see McCracken and Abraham (2005) and Asinari (2005)). Such these attempts are based on either a passive scalar model or a direct discretization of BGK-type models derived from the continuous kinetic theory. For example, the model of Luo and Girimaji (2003) and its subsequent modification by McCracken and Abraham (2005) are discrete velocity formulations of the Sirovich model (Sirovich (1962)). However, it is well known that the Sirovich model obeys neither the H-theorem nor the indifferentiability principle (i.e., it does not reduce to the single-component BGK fluid when the species become mechanically equivalent, see, e.g. Andries *et al.* (2002)). A physically sound modeling approach for approximating the mixture collision term is thus needed in any discrete velocity formulation. Recently, a new approach to model kinetic equations has been developed (Gorban and Karlin (1994); Levermore (1996); Ansumali *et al.* (2005); Gorban and Karlin (2005)). The basic idea (Gorban and Karlin (1994)) is a model representation on the fast-slow decomposition of motions near quasi-equilibrium states. Therein it was proposed that the relaxation to the equilibrium is modeled as a two-steps process, a "fast" relaxation from the initial state to the quasi-equilibrium f^* with a relaxation time τ_1, and a "slow" motion from the quasi-equilibrium state f^* toward the equilibrium. The fast relaxation is assumed in the BGK form, $\frac{1}{\tau_1}(f-f^*)$. The slow motion can also be approximated by a BGK term (Levermore (1996); Ansumali *et al.* (2005)) such that this process leads to the equilibrium f^{eq} with a second relaxation time $\tau_2 \geq \tau_1$. In this paper this model is extended to binary mixtures, and unlike the Sirovich's model, the approach ensures thermodynamic consistency (the H-Theorem is satisfied, Gorban and Karlin (1994)) as well as the indifferentiability principle. Furthermore, the lattice Boltzmann models for mixtures face severe numerical instabilities at large mass ratios (McCracken and Abraham (2005)). Some of these instabilities can be attributed to the discretization used in the previous works (Luo and Girimaji (2003); McCracken and Abraham (2005)). We derive the second-order Lattice Boltzamnn scheme, and numerically show that the present model can simulate mixtures with arbitrarily mass ratios.

2 Model Description

The discrete-velocity kinetic equation for each component $j = A, B$ of a binary mixture can be written as:

$$\partial_t f_{j\,i} + v_{j\,i\,\alpha}\,\partial_\alpha f_{j\,i} = \Omega_{j\,i}, \tag{1}$$

where $i = 1, .. N$, with N number of the discrete lattice velocities $v_{j\,i\,\alpha}$ and the collision term is $\Omega_{j\,i}$. Hydrodynamic quantities such as the density ρ_j and the momentum density $J_{j\,\alpha}$, in the α direction ($\alpha = x, y, z$), of the individual components j are:

$$\rho_j = \sum_i f_{ji}, \qquad\qquad J_{j\alpha} = \sum_i f_{ji}\, c_{ji\alpha}, \tag{2}$$

respectively. Here $c_{ji\alpha} = v_{ji\alpha}/\sqrt{k_{\rm B}T_0/m_j}$ are reduced discrete velocities of the components and T_0 is the reference temperature. Along with the species densities, the total mass density $\rho = \rho_A + \rho_B$ and total momentum density, $J_\alpha = J_{A\,\alpha} + J_{B\,\alpha}$ are the invariant of the collision term. We propose to write the collision term as (Ansumali *et al.* (2005)):

$$\Omega_{j\,i} = \frac{1}{\tau_1}\left[f^*_{j\,i}\left(\rho_j, J_{j\,\alpha}\right) - f_{j\,i}\right] + \frac{1}{\tau_2}\left[f^{\rm eq}_{j\,i}\left(\rho_j, J_\alpha\right) - f^*_{j\,i}\left(\rho_j, J_{j\,\alpha}\right)\right], \tag{3}$$

The quasi-equilibrium population distribution function f^*corresponding to each component j is obtained by maximizing the entropy function under fixed ρ_j and $J_{j\,\alpha}$ (Karlin *et al.* (1999)). This implies that only those two variables are approaching slowly to equilibrium and all the other moments are assumed to equilibrate faster. The result of the minimization problem is immediately read off the equilibrium for a single-component fluid (Ansumali *et al.* (2003)):

$$f^*_{ji} = \rho_j W_i \prod_{\alpha=1}^{D}\left(2 - \sqrt{1 + 3\left(\frac{J_{j\alpha}}{\rho_j}\right)^2}\right) \times \left(\frac{2\left(\frac{J_{j\alpha}}{\rho_j}\right) + \sqrt{1 + 3\left(\frac{J_{j\alpha}}{\rho_j}\right)^2}}{1 - \left(\frac{J_{j\alpha}}{\rho_j}\right)}\right)^{c_{ji\alpha}}.$$

The equilibrium populations are a subset of f^* corresponding to the momentum of the mixture $\mathbf{J} = \mathbf{J}_{\rm A} + \mathbf{J}_{\rm B}$, that is:

$$f^{\rm eq}_{ji}(\rho_j, \mathbf{J}) = f^*_{ji}(\rho_j, \mathbf{J}). \tag{4}$$

This completes the model description and it is obvious that the standard BGK model for single-component fluid is recovered for $\tau_1 = \tau_2$ and $m_A = m_B$.

3 Hydrodynamic Limit

The balance equation for the locally conserved quantites can be written using kinetic Eq.(1) as:

$$\begin{aligned}
&\partial_t \, \rho + \partial_\alpha \, J_\alpha = 0 \\
&\partial_t \, (\rho_A - \rho_B) + \partial_\alpha \left((\rho_A - \rho_B) \, \frac{J_\alpha}{\rho} + 2 \, V_\alpha \right) = 0 \\
&\partial_t \, J_\alpha + \partial_\beta \, P_{\alpha \, \beta} = 0,
\end{aligned} \tag{5}$$

where the pressure tensor

$$P_{\alpha\beta} = P_{A \, \alpha \, \beta} + P_{B \, \alpha \, \beta} = \sum_{i,j} f_{ji} \, c_{ji\alpha} \, c_{ji\beta}, \tag{6}$$

and the diffusion velocity between the two components V_α is defined as:

$$V_\alpha = \mu_{AB} \left(\frac{J_{A \, \alpha}}{\rho_A} - \frac{J_{B \, \alpha}}{\rho_B} \right), \tag{7}$$

with $\mu_{AB} = \frac{\rho_A \rho_B}{\rho_A + \rho_B}$ the reduced mass.
In the hydrodynamic limit, the present model recovers the Navier-Stokes equation for the momentum and Stefan-Maxwell diffusion equation for the densities of species with the viscosity μ and diffusion D_{AB} coefficients:

$$\mu = n \tau_1 k_B \, T, \qquad D_{AB} = X_A \, X_B \frac{P}{\mu_{AB}} \, \tau_2, \tag{8}$$

where $X_j = \frac{n_j}{n}$ is the molar fraction of the component j, $n_j = \frac{\rho_j}{m_j}$ the number density, and $n = n_A + n_B$. The present model is restricted to $\tau_1 \leq \tau_2$. The implications of such a model on the Schmidt number Sc is:

$$Sc = \frac{\mu}{\rho D_{AB}} \leq \frac{Y_A Y_B}{X_A X_B}, \tag{9}$$

where $Y_j = \frac{\rho_j}{\rho}$ is the mass fraction of the component j.

4 Numerical Implementation

It is reminded that in the lattice Boltzmann scheme, Eq. (1) is discretized by applying the implicit trapezoidal rule between time t and $t + \delta t$ (over-

relaxation) as:

$$f_{ji}(\mathbf{x}+c_{ji}\,\delta t, t+\delta t) = f_{ji}(\mathbf{x},t) + \frac{\delta t}{2}\left[\Omega_{ji}(f(\mathbf{x},t)) + \Omega_{ji}(f(\mathbf{x}+c_{ji}\,\delta t, t+\delta t))\right] + O(\delta t^3). \tag{10}$$

This scheme is rendered explicit by introducing a local transformation through auxiliary functions g_{ji} such that:

$$g_{ji}(\mathbf{x},t) = f_{ji}(\mathbf{x},t) - \frac{\delta t}{2}\,\Omega_{ji}(f(\mathbf{x},t)). \tag{11}$$

Evaluating the moments of $g_{ji}(\mathbf{x},\mathbf{t})$ from Eq. (11) for the collision model under consideration yields:

$$\begin{aligned} \rho_j(f) &= \rho_j(g), \qquad J_\alpha(f) = J_\alpha(g), \\ J_{j\alpha}(f) &= \frac{\frac{\delta t}{2\tau_2} J_{j\alpha}(g) + \frac{\rho_j}{\rho} J_\alpha(g)}{1+\frac{\delta t}{2\tau_2}}. \end{aligned} \tag{12}$$

The momentum $J_{j\alpha}$ of each individual species differs in the two distribution functions. This happens because species momentum is not conserved by the collision term (a general feature of collision models for mixtures). The difference between $J_{j\alpha}(f)$ and $J_{j\alpha}(g)$ vanishes when the two masses are the same ($m_\mathrm{A} = m_\mathrm{B}$), but becomes non-negligeble when the mass ratio becomes large. This effect of discreteness, which leads to a redefinition of the non-conserved moments, is overlooked in previous works and led to lattice Boltzmann methods that were of first order accuracy (McCracken and Abraham (2005) and Luo and Girimaji (2003)). By substituting in Eq. (10):

$$g_{ji}(\mathbf{x},t+\delta t) = g_{ji}(\mathbf{x},t) - \omega_1\left(g_{ji}(\mathbf{x},t) - f^*(\rho_j,J_j))\right) - \omega_2\left(f^*_{ji}(\rho_j,J_j) - f^{\mathrm{eq}}_{ji}(\rho_j,J)\right), \tag{13}$$

with: $\omega_1 = \frac{2\delta t}{2\tau_1+\delta t}$ and $\omega_2 = \omega_1\frac{\tau_1}{\tau_2}$. This discretization scheme allows for trasforming the initial implicit problem in f into an explicit equation for g. It is noted that in order to evaluate f^{eq} and f^*, moments must be computed using Eq. (12). Moreover, the time integration scheme is second order accurate.

In general, any space discretization can be used to solve Eq. (13). However, in order to keep the simplicity and computational advantages of the LB spacial integration scheme, the square root of the mass ratio was chosen to be an integer. This approach circumvents complicated interpolation schemes to calculate the moments from one grid to the other. The speed of sound for the

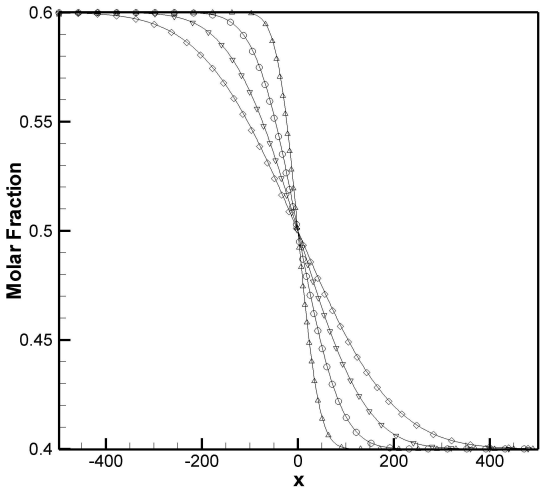

Fig. 1. Diffusion of a binary mixture. Initial molar concentration $60\%A \div 40\%B$ for $x < 0$ and $40\%A \div 60\%B$ for $x > 0$, mass ratio $\frac{m_A}{m_B} = 100$, and $\frac{\mu}{D} = 0.5$. Symbols LB predictions: up triangles time step 500; circles time step 2000; down triangles time step 5000, and diamonds time step 10000. Continuous lines: corresponding analytical solution.

species j is given by: $c_s^j = \sqrt{\left(\frac{k_B T_0}{m_j}\right)}$. In the LB formulation the time step is defined as: $dt = \frac{dx}{c_s}$, with dx lattice spacing. In order to have the same time step for both components during the calculations, two different lattice grids have to be used and the corresponding lattice spacing ratio is related to the ratio of the sound speeds of the two components, *i.e.* to the inverse of the square root of the mass ratio: $\frac{dx_A}{dx_B} = \frac{c_s^A}{c_s^B} = \sqrt{\frac{m_B}{m_A}}$. This implies the heavier component will have a finer grid or that the lighter component is diffusing faster than the heavier (Graham effusion law).
The model was tested by simulating the time evolution of the diffusion of two binary mixtures having a different component concentrations and comparing with the corresponding analytical solution (Incropera-DeWitt (2002)). Figure 1 shows the agreement between the LB calculations and the corresponding analytical solution for the larger mass ratio simulated.

A new Lattice Boltzmann model based on the quasi-equilibrium formulation for binary mixtures is developed, that, despite its simplicity (the implementation on top of the standard LBGK code is straightforward), is free of the drawbacks of previous models, is thermodynalically consistent and can accomodate high mass ratios within a wide range of the Schmidt numbers.

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