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# Multi-component lattice Boltzmann models for accurate simulation of flows with wide viscosity variation

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ABSTRACT

Multi-component lattice Boltzmann models operating in a wide range of fluid viscosity values are developed and examined. The algorithm is constructed with the goal to enable engineering applications without sacrificing simplicity and computational efficiency present in the original Shan–Chen model and D3Q19 lattice scheme. Boundary conditions for modeling friction and wettability effects are developed for discrete representation of surfaces within a volumetric approach, which results in accurate flow simulation in complex geometry. Numerical validation of our models includes comparison to previous studies and analytical solutions. The results are shown to be robust and accurate up to an extremely small kinematic viscosity value of 0.0017 lattice units and the extremely high ratio of components' kinematic viscosities of hundreds and up to a thousand. This improvement is significant compared to previous studies with Shan–Chen model [1,25,26], in which reasonable accuracy was kept only at the viscosity ratio up to 10 in the Poiseuille flow and the fingering simulation.



## 1. Introduction

The dynamics of multi-component flow commands considerable attention in many fields of physics and engineering due to its fundamental importance and industrial applications. In the recent decades, computational simulation has become a powerful tool to study multi-component flow, with the lattice Boltzmann method gaining popularity among numerous numerical techniques because it combines the microscopic and macroscopic approaches, its adaptability for complex geometry, and computational efficiency.

For the engineering applications, the adequate account of fluid properties such as viscosity and surface tension is required. If those can be varied at multiple resolutions and simulated Mach numbers without sacrificing accuracy and stability, one can accurately simulate a variety of systems within the appropriate range of characteristic non-dimensional parameters such as the Bond, Capillary, and Weber numbers, which is usually important for the multi-component flow. In particular, maintaining accuracy and stability of the simulation for a wide range of fluid viscosity variation is a very important functionality required for simulation of many flows, such as flow through the rock where numerical matching of the Capillary number may be necessary for accurate prediction of industrially important parameters.

One of the most popular multi-component LB models is known as the Shan–Chen (SC) model or, including its generalizations, the pseudo-potential model. While widely used, this model operates in a very limited range of viscosity values. For an example, in Ref. [1] it is reported that the original SC model is only stable within the viscosity ratio between components varying up to 5. While a recent enhancement described in [2] improves the stable viscosity ratio all the way into the range up to 1000, the model of Ref. [2] is too complicated to deliver computational efficiency and universality. In particular, its enhanced isotropy requires increased stencils which causes high computational cost and complicates application in arbitrarily complex geometry, while the multiple relaxation time scheme hurts implementation and performance. In the present study, the further development of SC model is driven by requirements of engineering applications. In particular, retaining the single-relaxation time scheme and the fourth isotropy order which can be naturally achieved by D3Q19, we modify the collisional operator in order to better control instabilities. We also introduce boundary conditions using a volumetric-based approach for modeling the friction and wettability effects.

This paper is organized as follows. In Section. 2, our modeling approach is discussed and some details of our LB models are presented. The comprehensive testing aimed at validating

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the model for engineering application requirements is described in Section. 3. These tests include a static droplet in free space, a multi-component Poiseuille flow, a slug between flat plates, a droplet on an inclined wall, 1% mixture flow in packed spheres, displacement of a slug from a channel, and fingering. In Section. 4, we summarize our observations and conclusions. In all cases of this study, density ratio between components is set as 1.

## 2. Lattice Boltzmann models for immiscible fluids

An inter-particle lattice Boltzmann model for immiscible fluids with wide viscosity range is introduced. The model is based on the Shan–Chen model [3,4] and its recent advancements [5,7–10]. The algorithm for bulk solver is presented first and followed by boundary conditions including surface friction and wetting condition on arbitrary geometry.

The lattice Boltzmann (LB) equation for multi-component fluid is:

$$f_i^\alpha(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) - f_i^\alpha(\vec{x},t) = \mathcal{C}_i^\alpha + \mathcal{F}_i^\alpha, \tag{1}$$

where $f_i^\alpha$ is the density distribution function of fluid component $\alpha$ and $\vec{c}_i$ is the discrete particle velocity. Henceforth, for simplicity, binary fluid is considered, namely $\alpha = \{1,2\}$, although the framework of this study can be extended to arbitrary number of components. The D3Q19 [11] lattice model with the fourth order lattice isotropy is chosen in this study. The term $\mathcal{F}_i^\alpha$ is associated with inter-component interaction force and its details are discussed in the follows. The collision operator $\mathcal{C}_i^\alpha$ is the Bhatnagar–Gross–Krook type,

$$\mathcal{C}_i^\alpha = -\frac{1}{\tau_{mix}}(f_i^\alpha - f_i^{eq,\alpha}). \tag{2}$$

Here, $f_i^{eq,\alpha}$ is the equilibrium distribution function for the Stokes flow with the third order expansion in $\vec{u}$ ,

$$f_i^{eq,\alpha} = \rho_\alpha w_i\left[1 + \frac{\vec{c}_i\cdot\vec{u}}{T_0} + \frac{(\vec{c}_i\cdot\vec{u})^3}{6T_0^3} - \frac{\vec{c}_i\cdot\vec{u}}{2T_0^2}\vec{u}^2\right], \tag{3}$$

where $T_0 = 1/3$ and $w_i$ denote the lattice temperature and isotropic weights in D3Q19, respectively. The density of the component $\alpha$, $\rho_\alpha$, and the mixture flow velocity, $\vec{u}$, are defined as,

$$\rho_\alpha = \sum_i f_i^\alpha, \quad \rho = \sum_\alpha \rho_\alpha = \sum_\alpha\sum_i f_i^\alpha,$$
$$\vec{u^\alpha} = \sum_i \vec{c}_i\cdot f_i^\alpha/\rho_\alpha, \quad \vec{u} = \sum_\alpha\sum_i \vec{c}_i\cdot f_i^\alpha/\rho. \tag{4}$$

The relaxation time $\tau_{mix}$ in Eq. (2) relates to the kinematic viscosity of the mixture of components, $\nu_{mix}$, as

$$\tau_{mix} = (\nu_{mix}/T_0) + 1/2, \tag{5}$$

$$\nu_{mix} = p\nu_1 + (1-p)\nu_2, \tag{6}$$

where $\nu_1$ and $\nu_2$ are kinematic viscosities of the first and second components. Here $p$ is a smooth function of $\rho_1$ and $\rho_2$, which ranges from 0 to 1. One of the simplest forms of such $p$ is a linear function of $\rho_1/(\rho_1+\rho_2)$. Following the conventional way [3,4], the inter-component force, $\vec{F}^{\alpha,\beta}$, between component $\alpha$ and $\beta$ is defined as,

$$\vec{F}^{\alpha,\beta}(\vec{x}) = G\rho_\alpha(\vec{x})\sum_i w_i\vec{c}_i\rho_\beta(\vec{x}+\vec{c}_i\Delta t), \tag{7}$$

for $\alpha\neq\beta$ and $\vec{F}^{\alpha,\beta}(\vec{x}) = 0$ for $\alpha=\beta$. When the interaction strength $G$ is negative, repulsive force acts between components and yields the separation. Following the manner in [5], this inter-component force is implemented to the forcing term $\mathcal{F}_i^\alpha$ in Eq. (1). The acceleration of the component $\alpha$, $\vec{g}_\alpha$, originated from $\vec{F}^{\alpha,\beta}$ is defined by $\vec{g}_\alpha = \sum_\beta \vec{F}^{\alpha,\beta}/\rho_\alpha$. The resulting fluid velocity $\vec{u}_F$ is defined as the velocity averaged over pre- and post- collision steps and written as,

$$\vec{u}_F = \vec{u} + \vec{g}\Delta t/2, \qquad \vec{g} = \sum_\alpha \vec{g}_\alpha\rho_\alpha/\rho. \tag{8}$$

In what follows, this quantity $\vec{u}_F$ is called simply *velocity*.

In order to enhance stability and accuracy when $\tau_{mix}$ is not close to 1, effects from the non-equilibrium state are regulated. After rearrangement of Eq. (1), one obtains,

$$f_i^\alpha(\vec{x}+\vec{c}_i\Delta t, t+\Delta t) = f_i^{eq,\alpha} + \left(1-\frac{1}{\tau_{mix}}\right)f_i^{'\alpha} + \mathcal{F}_i^\alpha. \tag{9}$$

The function $f_i^{'\alpha}$ is the nonequilibrium particle distribution for each fluid component. If $f_i^{'\alpha}$ takes the standard BGK form $f_i^\alpha - f_i^{eq,\alpha}$ and $\tau_{mix}$ is away from 1, one suffers from the instability caused by unphysical noise and numerical artifacts of the LB model. To address this issue, a collision procedure regarding $f_i^{'\alpha}$ is regulated by,

$$f_i^{'\alpha} = \Phi^\alpha : \Pi^\alpha. \tag{10}$$

Here $\Phi$ is a regularization operator that uses Hermite polynomials and $\Pi^\alpha$ is the nonequilibrium part of the momentum flux [6]. The basic concept of regularized collision procedure can be found in [7–10,12] i.e.

$$\Phi^\alpha = \frac{w_i}{2T^2}(\vec{c}_i\vec{c}_i - TI),$$
$$\Pi^\alpha = \sum_l \vec{c}_l\vec{c}_l\left(f_l^\alpha - f_l^{eq,\alpha}\right). \tag{11}$$

To better achieve noslip wall boundary condition on arbitrary geometries, an extension of the volumetric boundary condition proposed by Chen et al. in 1998 [13–16] is utilized. In this method, after boundary surfaces are discretized into linear surface facets in two dimension or triangular polygons in three dimension, the incoming and outgoing particles based on those facets or polygons are calculated in a volumetric way obeying the conservation laws. The extension of this method for various types of the boundary condition on arbitrary geometry has been studied. More details can be found in [13]. To reduce numerical smearing in near surface region, especially when physical viscosity is small and resolution is coarse, surface scattering model presented in [14] is crucial. Our simulations of the single component flow have demonstrated the superior of this boundary condition model at low viscosity and resolution. Results will be reported in a separate paper.

To realize surface wetting conditions, the inter-component interaction force in Eq. (7) is extended to the interaction force between wall and fluid particles, $\vec{F}_w^{\alpha,\beta}$, as,

$$\vec{F}_w^{\alpha,\beta}(\vec{x}) = G\rho_\alpha(\vec{x})\sum_i w_i\vec{c}_i\rho_\beta^{'}(\vec{x}+\vec{c}_i\Delta t), \tag{12}$$

for $\alpha\neq\beta$ and $\vec{F}_w^{\alpha,\beta}(\vec{x}) = 0$ for $\alpha=\beta$. $\rho_\beta^{'}$ is equivalent to the fluid density $\rho_\beta$ in the bulk region. And near the wall it is computed using fluid density and assigned solid density $\rho_\beta^s$, which is the wall potential for controlling the contact angle. This computation is performed so that the transition of $\rho_\beta^{'}$ is smooth [13] and the local momentum is conserved in bulk regions.

This volumetric wettability scheme has sufficient isotropy for keeping a droplet stable on the inclined wall to fluid lattices [17]. The wall potential for components, $\rho_1^s$ and $\rho_2^s$, are controlled with a single parameter $\rho^s$ so that if one of $\rho_1^s$ and $\rho_2^s$ is positive then the other one is set to 0.

## 3. Validations

In this section, using the LB models described in the previous section, a set of test cases, which are necessary for the engineer-

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