Thermal Lattice Boltzmann Method for Liquid-Gas Two-Phase Flows in Two Dimension

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A lattice Boltzmann method (LBM) for two-phase nonideal fluid flows is proposed based on a particle velocity-dependent forcing scheme. The resulting macroscopic dynamics via the Chapman-Enskog expansion recover the full set of thermohydrodynamic equations for nonideal fluids. Numerical verification of fundamental properties of thermal fluids, including viscosity, thermal conductivity, and surface tension, agrees well with theoretical predictions. Direct numerical simulations of two-phase phenomena, including phase-transition, bubble deformation and droplet falling and bubble rising under gravity are carried out, demonstrating the applicability of the model.

Key Words: Multi-Phase Flow, Computational Fluid Dynamics, Numerical Analysis, Lattice Boltzmann Method, Liquid-Gas Two-Phase Flows, Heat Flow in Multiphase Systems

1. Introduction

The study of multiphase flows is a formidable challenge due to complex surface phenomena and it is important for fundamental sciences and for engineering applications, including boiling physics, oil recovery, geophysical flows, bio-mechanical flows, and combustion. The one-component two-phase flow, such as the water-vapor flow, is a highly complex nonlinear phenomenon, including thermal-hydraulics, phase transition, bubble and droplet dynamics coupled with interface interactions. It is a laborious task to solve the macroscopic equations describing the processes in two-phase flow. Recently, several numerical methods have been proposed for simulating the two-phase flows based on mesoscopic dynamics. In particular, the lattice Boltzmann method (LBM)(1), an extension of the lattice gas automation method (LGA)(2), has received considerable attention as an alternative and promising numerical scheme for simulating fluid flows(3),(4) involving interfacial dynamics and complex boundaries. Unlike conventional numerical schemes based on macroscopic equations, the LBM is based on microscopic and mesoscopic kinetic equations. The fundamental idea of the LBM is to construct simplified kinetic models, incorporating the essential physics of microscopic or mesoscopic processes, so that the macroscopic averaged properties obey the desired macroscopic equations.

The kinetic nature of the LBM provides features distinct from other numerical methods. The convection operator of the LBM in phase space (or velocity space) is linear. This attractive feature originates from kinetic theory, and contrasts with non-linear convection terms in other approaches that use a macroscopic representation. The multi-scale expansion together with the collision process in the LBM recovers the non-linear macroscopic advection. Another feature is that the LBM only requires a small set of velocities in phase space. Since only one or two speeds and a few moving directions are used in the LBM, a transformation from the microscopic distribution function to macroscopic quantities is extremely simple and consists of no more than arithmetic calculations. Moreover, the parallel nature of the LBM affords easy implementation of efficient simulations on massively parallel computers.

In the last several years, the LBM has successfully been applied to multiphase fluid flows(5) – (9). Gunstensen et al. proposed an LBM model for solving two-component fluid flows based on the idea of colored particles in the immiscible lattice gas (ILG) model(5). Grunau et al. extended this model by including density and viscosity variations of
fluid components\textsuperscript{(6)}. Shan and Chen\textsuperscript{(10)} used interparticle potentials for surface ideal separation and Swift et al. directly introduced the nonideal pressure tensor into the LBM using a free energy formulation\textsuperscript{(11)}. However, all above models are essentially valid for isothermal systems, i.e., only mass conservation and momentum conservation are taken into consideration. The dynamics of the temperature distribution is essential for two-phase problems in which the fluid motion couples with heat transfer. To simulate two-phase thermal-hydraulics, it is crucial to improve the two-phase LB model by including the dynamic temperature.

Thermohydrodynamic LB models for ideal gases have been proposed by Alexander et al.\textsuperscript{(12)}, Qian\textsuperscript{(13)}, Shan\textsuperscript{(14)} and He et al.\textsuperscript{(15)} In these models, the internal energy or temperature is introduced using multiple particle velocities and the energy equation is obtained through choosing proper local equilibrium distribution functions. However, these LB models can be numerically unstable for certain parameter domains\textsuperscript{(16)}, and only flows with a narrow temperature range can be simulated. The numerical instability can be relaxed by introducing a finite differencing of the lattice Boltzmann equations, leading to a finite difference lattice Boltzmann method (FDLBM)\textsuperscript{(17)}.

Although the LBM for isothermal two-phase flows and for thermodynamics of ideal gases have been independently proposed and have been successfully applied to several simulations, it is difficult to combine energy conservation with a two-phase flow system with only distribution function for one component\textsuperscript{(14),(18),(19)}. A thermodynamically consistent lattice Boltzmann models with one distribution function for nonideal gases is theoretically derived from the Enskog equation (the modified Boltzmann equation for dense gases). This LB model, however, doesn’t succeed to provide simulation results of two-phase flows\textsuperscript{(20),(21)}. In most existing LB models, the correct form of the continuum equation for nonideal fluid can be obtained, but the energy conservation is not satisfied\textsuperscript{(22),(23)}.

In this paper we present a LB model capable of simulating the continuity, momentum and energy equations simultaneously for thermodynamic two-phase flows. In section 2, we present a detailed description of the LBM model, which leads to a nonideal pressure tensor. The development of a reliable LB model for two-phase thermal system will allow us to simulate heat transfer and surface phenomena simultaneously. In section 3, we discuss the numerical discretization of the LBM equations and the implementation of boundary conditions. In section 4 the transport coefficients, including viscosity and thermal conductivity, are verified by numerical experiments for Poiseuille flow and Couette flow. A quantitative test of Laplace’s law is given in this section. In section 5, several simulations, including spontaneous phase transition and bubble and droplet deformation will be shown to demonstrate the applicability of this model. Finally, in section 6, we discuss the limitation of the current model.

2. The Lattice Boltzmann Method

In this paper, the LBM will deal with the following continuity, momentum, and energy equations for thermodynamic nonideal flows:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_\alpha}{\partial x_\alpha} = 0, \quad (1)
\]

\[
\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial x_\beta} = \frac{\partial P_{a\beta}}{\partial x_\beta} + \frac{\partial}{\partial x_\beta} \left[ \rho \frac{\partial u_\gamma}{\partial x_\gamma} \right] - \frac{\partial \rho g_\alpha}{\partial x_\alpha} + \rho g_\alpha, \quad (2)
\]

\[
\frac{\partial \rho e}{\partial t} + \frac{\partial \rho e u_\alpha}{\partial x_\alpha} = -P_{a\beta} \frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial}{\partial x_\alpha} \left[ \rho \frac{\partial T}{\partial x_\alpha} \right] + \rho \frac{\partial}{\partial x_\alpha} \mu \left( \frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta} \right), \quad (3)
\]

where \( \rho \) is the density, \( u \) is the local velocity, \( e \) is the internal energy, \( T \) is the temperature, \( P_{a\beta} \) is the pressure tensor, \( g_\alpha \) is a gravitational constant, and \( \mu, \lambda, \kappa_\gamma \) are the shear viscosity, second viscosity, and thermal conductivity, respectively. The Greek subscripts \( \alpha, \beta, \gamma \) denote the space directions in Cartesian coordinates. The pressure tensor in a nonuniform fluid, \( P_{a\beta} \), is derived from the van der Waals-Cahn-Hilliard free energy\textsuperscript{(11),(23)}:

\[
P_{a\beta} = \left[ p - \kappa_\gamma \rho \nabla^2 \rho - \frac{\kappa_\gamma}{2} |\nabla \rho|^2 \right] \delta_{a\beta} + \kappa_\sigma \left( \frac{\partial \rho}{\partial x_\alpha} \right) \left( \frac{\partial \rho}{\partial x_\beta} \right), \quad (4)
\]

where \( p \) is the pressure of the fluid:

\[
p = \frac{\rho T}{1 - b_\gamma} - a_\gamma^2, \quad (5)
\]

given by an equation of state. Here, \( a_\gamma^2 \) represents the effect of long-range attractive molecular forces; \( b \) represents the influence of short-range repulsive forces; \( \kappa_\gamma \) is the surface tension parameter which controls the strength of the surface tension, and \( \delta_{a\beta} \) is the Kronecker delta function. The van der Waals equation of state is a reasonable model for both liquid and vapor properties\textsuperscript{(24)}. Although in general this equation of state can not give quantitative features of real liquids, it is a useful model to demonstrate fundamental phenomena in multiphase fluids, such as phase change and behavior at the critical point. Direct numerical simulation of Eqs. (1)–(5) is difficult because the equation of state is nonideal, giving rise to phase transition and surface phenomena. The use of the LBM makes it possible to model the physics described by these equations.

The LBM starts from the following Boltzmann equation for the discrete velocity distribution function, \( f_{\sigma x} \), on a discrete lattice:

\[
\frac{\partial f_{\sigma x}}{\partial t} + u_{\sigma x} \cdot \nabla f_{\sigma x} = \Omega_{\sigma x}, \quad (i=1,2,\cdots,N), \quad (\sigma=0,1,2,\cdots,M), \quad (6)
\]
where \( \mathbf{e}_{r,i} \) is the unit velocity vector along the \( r \)th direction in space, \( \sigma \) is the velocity suffix, \( N \) is the number of directions of velocity, \( M \) is the number of speeds, and \( Q_{r,i} \) is the collision operator.

When a single-time relaxation approximation, \( Q_{r,i} = -\frac{f_{r,i} - f_{r,i}^{(0)}}{\tau \epsilon} \), is applied to Eq. (6), we obtain the standard lattice BGK (LBGK) equation in nondimensional form\(^{(4),(25)}\), where \( \tau \) is the relaxation time, \( f_{r,i}^{(0)} \) is the local equilibrium distribution, and \( \epsilon \) is a small parameter, proportional to the Knudsen number.

From the above LBGK equation, we construct a mesoscopic two-phase flow model by adding a forcing term, \( F_{r,i} \), and a gravity term, \( G_{r,i} \). The thermohydrodynamics are included by adding extra velocities in the definition of the kinetic energy or temperature. The mesoscopic evolution equation for two-phase thermohydraulics is written as follows:

\[
\frac{\partial f_{r,i}}{\partial t} + \mathbf{e}_{r,i} \cdot \nabla f_{r,i} = -\frac{f_{r,i} - f_{r,i}^{(0)}}{\tau \epsilon} + F_{r,i} + G_{r,i},
\]

where \( F_{r,i} \) and \( G_{r,i} \) will be determined later for obtaining appropriate forms of the pressure tensor and the gravitational field at the macroscopic level, respectively.

Thermohydrodynamical quantities, including the density \( \rho \), momentum \( \rho \mathbf{u}_i \), and the internal energy \( \epsilon \), are defined through the moments of the distribution function, \( f_{r,i} \):

\[
\begin{align*}
\sum_{r,i} f_{r,i} &= \rho, \\
\sum_{r,i} f_{r,i} (\mathbf{e}_{r,i})_0 &= \rho \mathbf{u}_i, \\
\sum_{r,i} \frac{1}{2} |\mathbf{e}_{r,i} - \mathbf{u}|^2 f_{r,i} &= \rho \epsilon.
\end{align*}
\]

For simplicity, in this paper we use the three-speed two-dimensional hexagonal lattice: one rest particle, \( (\mathbf{e}_0)_0 = 0 \), and two kinds of moving particles with nonzero velocity vectors: \( \mathbf{e}_{r,i} = \sigma \left[ \cos \left( \frac{2 \pi (i-1)}{6} \right), \sin \left( \frac{2 \pi (i-1)}{6} \right) \right] \) \((i = 1, \ldots, 6)\), \((\sigma = 1, 2)\), where \( \sigma \) denotes the magnitude of particle velocity.

In order to obtain the macroscopic equations from Eq. (7), we utilize the Chapman-Enskog method or the multi-scale expansion, assuming\(^{(25)}\)

\[
f_{r,i} = f_{r,i}^{(0)} + \epsilon f_{r,i}^{(1)} + \epsilon^2 f_{r,i}^{(2)} + \cdots.
\]

Applying the standard Chapman-Enskog procedure to Eq. (7)\(^{(25)}\), we obtain the continuity equation,

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \mathbf{u}_i)}{\partial x_i} = \sum_{r,i} [F_{r,i} + G_{r,i}],
\]

and the momentum equation,

\[
\frac{\partial (\rho \mathbf{u}_i)}{\partial t} + \frac{\partial (\rho \mathbf{u}_i \mathbf{u}_i)}{\partial x_i} = \frac{\partial (\rho \mathbf{u}_i \mathbf{e}_{r,i} + \epsilon G_{r,i})}{\partial x_i} + \frac{\partial (\rho \mathbf{u}_i \mathbf{e}_{r,i} + \epsilon G_{r,i})}{\partial x_i},
\]

and the energy equation,

\[
\frac{\partial \rho \epsilon}{\partial t} + \frac{\partial (\rho \mathbf{u}_i \epsilon)}{\partial x_i} + \frac{\partial (\rho \mathbf{u}_i \mathbf{u}_i \epsilon)}{\partial x_i} = \frac{\partial (\rho \mathbf{u}_i \mathbf{u}_i \epsilon)}{\partial x_i} + \frac{\partial (\rho \mathbf{u}_i \mathbf{e}_{r,i} + \epsilon G_{r,i})}{\partial x_i}.
\]

where the momentum flux tensor, \( \Pi_{\alpha \beta}^{(i)} \), and the heat flux, \( Q_a^{(i)} \), with \( l = 0, 1 \), are defined as

\[
\Pi_{\alpha \beta}^{(0)} = \sum_{r,i} \frac{f_{r,i}^{(0)} (\mathbf{e}_{r,i})_0 (\mathbf{e}_{r,i})_0}{\tau \epsilon},
\]

\[
Q_a^{(0)} = \frac{1}{2} \sum_{r,i} f_{r,i}^{(0)} (\mathbf{e}_{r,i} - \mathbf{u})^T (\mathbf{e}_{r,i} - \mathbf{u}) (\mathbf{e}_{r,i})_0,
\]

The equilibrium distribution function, \( f_{r,i}^{(0)} \), is given by a truncated power series in the local velocity \( \mathbf{u} \) assuming \( \mathbf{u} \ll 1 \):

\[
f_{r,i}^{(0)} = \rho (A_{0} + B_{\sigma} \mathbf{e}_{r,i} \cdot \mathbf{u} + C_{\sigma} (\mathbf{e}_{r,i} \cdot \mathbf{u})^2 + D_{\sigma} \mathbf{u}^2 + E_{\sigma} (\mathbf{e}_{r,i} \cdot \mathbf{u})^3 + F_{\sigma} (\mathbf{e}_{r,i} \cdot \mathbf{u}) \mathbf{u}^2),
\]

where the coefficients, \( A_{0}, B_{\sigma}, C_{\sigma}, D_{\sigma}, E_{\sigma}, F_{\sigma} \), are assumed to be the same as in Ref. (10).

\[
A_{0} = 1 - \frac{5 \epsilon}{2} + 2 \epsilon^2, \quad A_{1} = \frac{4 \epsilon (1 - \epsilon)}{9}, \quad A_{2} = \frac{8 \epsilon (4 \epsilon - 1)}{36},
\]

\[
B_{1} = \frac{4 (1 - \epsilon)}{9}, \quad B_{2} = \frac{(4 \epsilon - 1)}{36}, \quad C_{1} = \frac{2 (1 - \epsilon)}{9},
\]

\[
C_{2} = \frac{6 \epsilon - 1}{72}, \quad D_{0} = \frac{5}{4} + \frac{2 \epsilon}{9}, \quad D_{1} = \frac{2 (1 - \epsilon)}{9},
\]

\[
D_{2} = \frac{(4 \epsilon - 1)}{72}, \quad E_{1} = \frac{4}{27}, \quad E_{2} = \frac{1}{108},
\]

\[
F_{1} = 0, \quad F_{2} = 0.
\]

After simple algebra, the above distribution function yields the following fluxes:

\[
\Pi_{\alpha \beta}^{(0)} = \rho \mathbf{u}_i \delta_{\alpha \beta} + \rho \mathbf{u}_i \mathbf{u}_i, \quad \Pi_{\alpha \beta}^{(1)} = -\lambda \frac{\partial \mathbf{u}_i}{\partial x_\alpha} \delta_{\alpha \beta} + \rho \frac{\partial \mathbf{u}_i}{\partial x_\alpha}, \quad Q_{\alpha}^{(0)} = \rho \mathbf{u}_i \mathbf{u}_\alpha, \quad Q_{\alpha}^{(1)} = -\kappa T \frac{\partial T}{\partial x_\alpha},
\]

\[
+ \frac{\tau}{2} \sum_{r,i} \frac{f_{r,i}^{(0)} (\mathbf{e}_{r,i})_0 (\mathbf{e}_{r,i})_0}{\tau \epsilon} \mathbf{F}_{r,i} - 4 \epsilon \frac{\partial (\rho \mathbf{u}_i \mathbf{e}_{r,i} - P_{\alpha \beta})}{\partial x_\alpha} \frac{\partial \mathbf{u}_i}{\partial x_\alpha},
\]

where the shear viscosity, the second viscosity, and the thermal conductivity are given by \( \mu = (\rho \epsilon + \rho p) \tau / 2 \), \( \lambda = -(\rho \epsilon + \rho p \tau / 2, \kappa T = (\rho \epsilon + \rho p \tau) \tau \), respectively, and yield a Prandtl number, \( Pr = 0.5 \). After substituting Eqs. (17)–(20) into Eqs. (10)–(12), comparing with Eqs. (1)–(3), one obtains the constraints for \( F_{r,i} \) and \( G_{r,i} \):

\[
\sum_{r,i} F_{r,i} = 0, \quad \sum_{r,i} G_{r,i} = 0,
\]

\[
\sum_{r,i} F_{r,i} (\mathbf{e}_{r,i})_0 = \frac{\partial (\rho \mathbf{u}_i \mathbf{e}_{r,i} - P_{\alpha \beta})}{\partial x_\alpha}, \quad \sum_{r,i} G_{r,i} (\mathbf{e}_{r,i})_0 = \rho g_{\alpha},
\]
where $G_{cr}$, $H_{cr}$ and $a_p$ through $d_p$ are coefficients. For the three-speed model used in this paper and from the constraints, these coefficients can uniquely be obtained:

\[
\begin{align*}
    a_p &= -\frac{1}{15}, \\
    b_p &= d_p = \frac{\kappa}{15}, \\
    c_{p,1} &= \frac{2\kappa}{15}, \\
    c_{p,2} &= \frac{\kappa}{30}, \\
    G_1 &= \frac{20(1-\epsilon)}{3}, \\
    G_2 &= \frac{5(4\epsilon - 1)}{12}, \\
    H_1 &= \frac{10}{3}, \\
    H_2 &= \frac{5}{6}.
\end{align*}
\]

In a thermal system, the second terms in Eqs. (21) and (22) are necessary in order to recover the energy equation of a nonideal fluid at the macroscopic level. Since the first and second terms contain first and second order tensors, respectively, $F_{cr}$ and $G_{cr}$ can contribute to the derivations of mass, momentum, and energy equations. In each derivation, the effects of the $F_{cr}$ and of $G_{cr}$ are suitably controlled by the coefficients, $G_{cr}$ and $H_{cr}$ in the equations, depending on the magnitude of velocity, $\sigma$. For instance, in the derivation of mass equation, the effect of the second term in Eq. (22) is set to zero. Likewise, the first term in Eq. (21) can be used to set the pressure tensor in the momentum equation and a term concerning thermal conductivity, and the second can give the appropriate pressure tensor in the energy equation.

3. Discretization of Lattice Boltzmann Scheme

The LBM has several advantages over the lattice gas method, including no statistical noise, satisfying the Galilean invariance and no spurious invariants\(^{(3)}\). A drawback of the LB method is that the scheme could be numerically unstable for high Reynolds number flows and for thermal problems. The numerical instability induced by the use of LBGK in the simulation of two-D and three-D flows has been studied\(^{(25)}\). In general, numerical stability requires that the time step and spatial step satisfy the Courant-Friedrich-Levy (CFL) condition: $|\text{DE}| |\Delta t|/|\Delta x| < 1$. For the 13-velocity thermal model, the standard LBM does not satisfy this CFL condition for the velocity distribution function with speed $v_{\epsilon}^{(2)}$. With the Finite Difference Lattice Boltzmann Method (FDLBM), the stability can be ensured by relaxing the Lagrangian particle convection and by satisfying the CFL condition.

In this paper, the temporal discretization in Eq. (7) is calculated with a second order Runge-Kutta (or the modified Euler) method. The time evolution of particle distribution functions is derived using $f_{cr}(n+1/2) = f_{cr}(n) + \frac{1}{2} \Delta t(-\sigma_{cr} \nabla f_{cr} + G_{cr})$, where $f_{cr}(n+1) = f_{cr}(n) + \Delta t(-\sigma_{cr} \nabla f_{cr} + G_{cr})$, and $f_{cr}(n+1/2) = f_{cr}(n) + \Delta t(-\sigma_{cr} \nabla f_{cr} + G_{cr})$, where the superscripts $(n)$, $(n+1/2)$, $(n+1)$ are in units of $\Delta t$, and are given by $n = t/\Delta t$. A first order upwind scheme is appropriate for capturing steep gradients in interface problems\(^{(15)}\). To stably simulate two-phase flows, the convection term is discretized using the simplest upwind scheme: $\partial f_{cr}/\partial x = [f_{cr}(x,y) - f_{cr}(x-\Delta x,y)]/\Delta x$, for $\epsilon_2 = 0$, $\partial f_{cr}/\partial y = [f_{cr}(x,y) - f_{cr}(x,y)]/\Delta y$, for $\epsilon_2 < 0$. To verify viscosities and thermal conductivities for every phase, only the physical viscosity should survive. For numerical simulations without liquid-gas interfaces, spatial discretization can be obtained using a second order central difference scheme: $\partial f_{cr}/\partial x = D_x f_{cr} = [f_{cr}(x+\Delta x,y) - f_{cr}(x-\Delta x,y)]/(2\Delta x)$, $\partial f_{cr}/\partial y = D_y f_{cr} = [f_{cr}(x,y+\Delta y) - f_{cr}(x,y-\Delta y)]/(2\Delta y)$. Namely this second order spatial discretization is utilized in Poiseuille flow and Couette flow simulations.

Usually, boundary conditions in the LBM have been directly adopted from the lattice gas automaton method. The LBM has yielded no-slip boundary condition with “bounce-back” scheme, in which, after a particle reaches at a wall node, the particle reverses its velocity. This very simple way of handling boundary conditions, “bounce-back,” leads to mass conservation and succeeds in simulating fluid flows through porous media. Recently, however, this simple “bounce-back” method was found to give only first order accuracy, in spite of the second-order accuracy of the LBM\(^{(26)}\) away from boundaries. In this paper, for handling boundary condition for the distribution function, we use an “extrapolation scheme”\(^{(26)}\), which is second order accuracy. We assume that there is one additional layer of sites, beyond the boundary, inside the wall, and enforce the following condition each time step for the outside nodes before streaming:

\[
f_{cr}^{-1} = 2f_{cr} - f_{cr}^{-1},
\]

where $f_{cr}^{-1}$, $f_{cr}^0$, and $f_{cr}^1$ are the distribution functions on the outside layer, the wall layer, and the first layer inside the fluid, respectively.
4. Examination of Fundamental Properties of the Two-Phase LBM

The numerical experiments of fundamental properties are carried out for fluids in the liquid state and the vapor state. Each state can be determined by Maxwell construction for the van der Waals equation of state with the parameters \( a = 9/28 \), \( b = 2/21 \) (see Fig. 1). Although high density ratio between the vapor and the liquid is obtained by the decrease in temperature, the equation of state has minus pressure at the temperature less than 0.84375. To avoid instabilities induced by the minus pressure, we set the starting temperature 0.9, which is close to the critical temperature, \( T_c = 1.0 \). The starting liquid density is 5.767 (\( \Diamond \) in Fig. 1) and vapor density is 1.400 (\( \Box \) in Fig. 1) for a given temperature, \( T = 0.9 \).

In order to verify the momentum transport, we make use of the Poiseuille flow. The convection term in Eq. (7) is discretized using a second order central difference scheme. The parabolic velocity profile is obtained in Poiseuille flow under forcing and the viscosity is related to the velocity at channel center as

\[
\mu = \frac{W^2 \rho g_s}{8 \Delta u_0},
\]

where \( u_0 \) is the velocity at the channel center, and \( W \) is the channel width\(^{(12)}\). The viscosity can be inferred by measuring the velocity. This run is carried out with \( 64 \times 64 \) grid points. \( \Delta \lambda = \Delta y = 0.5 \), time step, \( \Delta t = 0.1 \), initial internal energy, \( \varepsilon = 0.9 \) and the gravity, \( g_s = 0.000075 \). Periodic boundary conditions are applied in the \( x \) direction and no-slip boundary conditions apply in the \( y \) direction. In Fig. 2, we show the dependence of viscosity on the relaxation time, \( \tau \). Figure 2 shows excellent agreement between the analytical solutions, \( \mu = (\rho \varepsilon + \rho) \tau/2 \), indicated by solid lines, and numerical solutions for the liquid (\( \times \)) and for vapor phases (\( + \)). For comparison with the present results, Fig. 2 indicates numerical results (\( \ast \)) with the simple pseudo potential LBM for two-phase flows proposed by Kato et al.\(^{(22)}\) for various values of \( \tau \). The shear viscosity for the pseudo potential LBM is given by, \( \mu = \rho \varepsilon \tau \). Although the pseudo potential LBM also shows that calculated results agree well with the analytical solutions for the vapor phase, it isn’t able to get solutions for liquid state using the second order central difference scheme due to numerical instability. By the modification of the fictitious forcing term, the proposed LB model becomes numerically more stable than the pseudo potential LBM. From the simulation result of Poiseuille flow, it is reasonable to conclude that the shear viscosity is correctly implemented and the momentum equation is correct up to second order in \( \varepsilon \).

To verify the thermal properties of the model, we simulate Couette flow, whose exact solution can be obtained. With a small temperature gradient, the normalized temperature distribution has analytic solution:

\[
T^* = \frac{T - T_0}{T_1 - T_0} = \frac{1}{2}(1 + y^*) + \frac{Br}{8}(1 - y^*^2),
\]

where \( y^* \) is the normalized distance from the center of the channel, \( Br \) is the product of the Prandtl and Eckert num-

![Fig. 1](image1)

Fig. 1 Isotherms (dashed lines) for the van der Waals equation of state for various temperatures in \( P - \rho \) coordinates. The solid line is the coexistence curve numerically determined by Maxwell’s equal area rule\(^{(24)}\). The densities of coexisting points at temperature \( T = 0.9 \) are 1.400 (\( \Diamond \)) and 5.767 (\( \Box \)) respectively. The points correspond to saturated vapor and liquid state. The temperature of the critical point is \( T_c = 1.0 \). The parameter values are \( a = 9/28 \), and \( b = 2/21 \).

![Fig. 2](image2)

Fig. 2 The measurement of viscosity as a function of \( \tau \) using the simulation of Poiseuille flow for coexisting phase states: vapor state (\( \rho = 1.400 \)), liquid state (\( \rho = 5.767 \)). The numerical solutions of vapor state (\( + \)) and of liquid state (\( \times \)) are compared with analytical solution (solid lines). Asterisks (\( \ast \)) show the numerical results for vapor state with the simple pseudo potential LBM\(^{(22)}\). The initial internal energy, \( \varepsilon = 0.9 \) and gravity \( g_s = 0.000075 \). The grid size, \( \Delta \lambda = \Delta y = 0.5 \), and time step, \( \Delta t = 0.1 \), are used in the simulation.
bers: \( Br = \frac{\mu u_0^2}{\kappa_T(T_1 - T_0)} \), and \( T_1 \) and \( T_0 \) are the temperatures of the top and bottom walls, respectively. The grid points are \( 32 \times 32 \), \( \Delta x = \Delta y = 0.5 \), and \( \Delta t = 0.01 \). The bottom wall is at rest and the top wall moves with speed \( u_0 = 0.1 \). The simulations are also carried out for liquid and vapor phases with the temperature of the bottom wall, \( T_0 = 0.900 \). The temperature of the top wall, \( T_1 \), equals to 0.901 for \( Br = 5.0 \), and equals 0.900 for \( Br = 10.0 \), respectively.

In Fig. 3, asterisks (•) and dots (○) show calculated temperature profiles with pseudo potential LBM proposed by Kato et al.\(^{(22)}\). The pseudo potential LBM doesn’t show fair agreement with the analytical solutions for any Brinkman numbers, because it can not derive the correct form of the energy equation for two-phase flows from the mesoscopic kinetic equation. In contrast very good agreement is seen in Fig. 3 (a) and (b) between the analytical and numerical solutions with the present model for both Brinkman numbers and for both densities. This result indicates that the proposed model is valid in simulating flows with thermal diffusion.

The third numerical test is to verify the surface tension or Laplace’s law at an interface for a two-phase fluid,

\[
\Delta P = \frac{\sigma_s}{R},
\]

where \( \Delta P \) is the pressure difference between the inside and outside of a single-component droplet, and \( R \) is radius of the spherical domain. Equation (28) indicates that \( \Delta P \) is proportional to the curvature of droplet, \( 1/R \). In this simulation, spatial discretization in Eq. (7) is calculated with the first order upwind scheme, and \( \Delta x = \Delta y = 0.5 \), \( \Delta t = 0.1 \), \( \tau = 0.16 \), and \( \kappa_s = 0.02 \). Figure 4 shows the numerical results are in reasonable agreement with Laplace’s law, and demonstrate the validity of the method for simulating two-phase flows in which the nonideal pressure tensor is an important factor.

5. Applications of the Two-Phase LBM

The two-phase flow is complicated by bubble and droplet deformation, collision, and coalescence. The proposed LB approach has the capability of reproducing the interesting phenomena. In order to substantiate its applicability, we perform four simulations: spinodal decomposition, distortion of bubble forced by shear stress, bubble dynamics forced by buoyancy, and droplet dynamics forced by gravity with heat transfer.

The first application is the spontaneous phase transi-

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Fig. 3 Simulation of Couette flow with heat transfer at coexisting states: (a) vapor state (\( \rho = 1.400 \)), (b) liquid state (\( \rho = 5.767 \)). Normalized Temperature \( T' = (T - T_0)/(T_1 - T_0) \) for Brinkman number, \( Br = 5.0 \) (•) and \( Br = 10.0 \) (○). The solid line is the analytical solution. Asterisks (•) and dots (○) show the numerical results with the simple pseudo potential LBM\(^{(22)}\). The bottom wall is at rest and the top wall moves at the constant speed \( u_0 = 0.1 \).

Fig. 4 Verification of Laplace’s law. The numerically measured pressure difference \( \Delta P \) is plotted as a function of \( 1/R \), where \( R \) is the radius of the droplet. The relaxation time \( \tau \) is 0.16, surface tension parameter \( \kappa_s \) is 0.02, and the temperature \( T \) is 0.900. The grid size, \( \Delta x = \Delta y = 0.5 \), the time step, \( \Delta t = 0.1 \) are used in the simulations.
tion induced by the thermodynamic instability of the van der Waals fluid. When the initial condition imposes densities in the unstable region, the phases will spontaneously separate into domains occupied by the coexisting phases. The initial state density, \( \rho \), is 3.33, and temperature, \( T = 9/10 \). The initial density fluctuation of 1\% is added to initiate the spinodal decomposition. This simulation was carried out using 256\times256 grid points. \( \Delta x = \Delta y = 0.5 \), and the time step, \( \Delta t = 0.1 \). The relaxation time, \( \tau = 0.16 \), and surface tension parameter, \( \kappa_s = 0.02 \). Figure 5 shows results of density distribution at different time steps. The variation of the density is illustrated with high density in black and low density in grey. As time evolves, the shape of the separated droplets gradually approaches a circle due to surface tension. Figure 6 shows the temperature distribution in the same simulation as Fig. 5. Comparing Fig. 5 with Fig. 6, it is seen that the temperature of the vapor is relatively higher than that of the liquid.

The next application is the bubble distortion under a shear stress generated by the walls moving in opposite direction. A circular bubble is initially surrounded by the liquid and is deformed by the shear stress in the liquid. The simulation uses 256\times256 grid points. \( \Delta x = \Delta y = 0.25 \), \( \Delta t = 0.05 \), \( \tau = 0.1 \), \( \kappa_s = 0.001 \). Periodic boundary conditions and moving wall boundary conditions are applied in the \( x \) direction and in the \( y \) direction, respectively. The top wall moves with constant velocity, \( u_1 = -0.1 \), and the bottom wall moves in the opposite direction with constant velocity, \( w_0 = 0.1 \). The initial conditions correspond to a null velocity everywhere except at the walls. The viscosity ratio \( \eta = \mu_G / \mu_L = 0.2428 \), where \( \mu_G \) and \( \mu_L \) are the viscosities of the gas and of liquid, respectively. The capillary number \( Ca = \mu_L \Gamma R / \sigma_s = 0.1386 \), where \( R \) is the radius of the bubble, \( \Gamma = 2(u_0 - u_1)/(255\Delta y) \) is the shear rate. Surface tension coefficient \( \sigma_s = 0.09395 \), which is calculated using Laplace’s law. Figure 7 shows a sequence of density distributions at different times. Letting the system evolve, we observe that a bubble becomes gradually deformed, stretched, and finally breaks up into two drops. Rallison indicates the analytical capillary number for breakup cri-
The critical value $Ca_c = 0.1387$. Just below $Ca_c$ predicted by the theoretical equation\textsuperscript{(27)}, the breakup behavior, so-called fracture, is observed in Fig. 7. This simulation carried out in two dimension should be carefully compared with the experimental or theoretical results. However, it seems to be quite all right to consider that this proposed LB model can calculate reasonable solutions for two-phase flows that other isothermal LB models succeeded. As noted by Inamuro et al.\textsuperscript{18}, the effect of the Reynolds number on drop deformation and breakup should be also investigated.

The third application is a bubble rising due to gravity. When a bubble exists in liquid in a gravitational field, buoyancy acts on it due to the static pressure difference between top and bottom of the bubble. The buoyancy makes the bubble rise opposite to the direction of the gravity. The simulation uses $256 \times 512$ grid points. $\Delta x = \Delta y = 0.25$, $\Delta t = 0.05$, $\tau = 0.1$, and $\kappa_s = 0.001$. Gravity, $g$, is $-0.00045$. Weber number $W$ and Reynolds number $Re$ are given by $We = \rho_l U_t^2 D/\sigma$ and $Re = \rho_l U_t D/\mu_l$, respectively. $D$ is the volume equivalent diameter of a bubble, $U_t$ is the terminal rising velocity. The surface tension, which is necessary to calculate the Weber number, is derived from Laplace’s law, Eq. (28). Figure 8 shows the time evolution of the density distribution with the average velocity distribution indicated by arrows. The bubble rises, deforming spherical to ellipsoidal shape, and finally it becomes oblate ellipsoidal cap. Circulating flow is found around the bubble. These results show that buoyancy can be reproduced by the proposed LB model. Ryskin et al.\textsuperscript{(28)} studied a general graphical correlation to predict the shape and terminal rising velocity of any bubble in terms of the dimensionless groups, $W$ and $Re$. The simulation results shown in Fig. 8 (a) and (b) are almost equal to computed results shown in the shape regime map in Ref. (28), which quantitatively agree with experimental results in Ref. (29). Compared with the results in Ref. (28), the deformation of the shape shown in Fig. 8 (c) and (d) are too large at the low values of $W$ and $Re$. It is not clear from these numerical results, but it is regarded as the cause that the present condition differs from that of Ref. (28). The temperature in this simulation is much higher than room temperature, and the bubble rises with phase transition between vapor
Fig. 7 Bubble distortion induced by shear. The snapshots are time evolution of the density distribution at $t = (a) 100, (b) 1000, (c) 2000, (d) 4000, (e) 4200, and (f) 4500$ (lattice unit). The grey color indicates vapor. The temperature, $T$, is 0.9 and densities are 1.400 and 5.767 for bubble and for the surrounding liquid, respectively. The relaxation parameter is 0.1, and surface tension parameter $\kappa_s$ is 0.001. The bottom wall moves with speed $u_1 = 0.1$ and the top wall moves in the opposite direction with speed $u_0 = -0.1$. $256 \times 256$ grid points are used in the simulation with grid size, $\Delta x = \Delta y = 0.25$ and time step $\Delta t = 0.05$.

Fig. 8 Simulation of a bubble rising due to gravity. The snapshots are bubble shapes and velocity distributions at $t = (a) 100, (b) 500, (c) 1000, and (d) 1500$ (lattice unit). Reynolds number $Re = 8.47$ (a), 12.52 (b), 9.39 (c), 14.91 (d), and Weber number $W = 2.02$ (a), 4.12 (b), 2.07 (c), 4.65 (d). The gravity $g_x$ equals $-0.00045$, the temperature $T$ is 0.9. Densities are 1.400 and 5.767 for bubble and for the surrounding liquid, respectively. The relaxation parameter $\tau$ is 0.1 and surface tension parameter $\kappa_s$ is 0.001. The simulation uses $256 \times 512$ grid points, $\Delta x = \Delta y = 0.25$, and time step $\Delta t = 0.05$. 

and surrounding liquid. It is cited as another cause that the pseudo fluid flows on the interface accelerate the deformation of the bubble.

The last simulation is liquid droplet deformation under gravity. The simulation uses $256 \times 256$ grid points. $\Delta x = \Delta y = 0.25$, $\Delta t = 0.05$, $\tau = 0.1$, $\kappa_s = 0.001$, $g_y = -0.0015$, temperature at walls, $T_0 = 1.0$, and the initial temperature of the droplet, $T = 0.88$. The density and velocity distribution are shown in Fig. 9, and the temperature distribution inside the droplet is plotted in Fig. 10. The simulations results presented here were not directly compared with experimental or analytical results, they demonstrate that the proposed lattice Boltzmann method has the capability to reproduce two-phase thermohydraulics.

![Simulation snapshots](image)

(a) $t = 50$
(b) $t = 200$
(c) $t = 250$
(d) $t = 400$

Fig. 9 Simulation of a droplet falling under gravity on a heated plate. The snapshots illustrate droplet deformation and velocity distributions at $t = (a) 100$, (b) 500, (c) 1000, and (d) 1500 (lattice unit). The gravity $g_y$ equals $-0.00015$. The initial densities are 5.767 and 1.400 for a droplet (black) and the surrounding vapor (grey), respectively. The initial temperature of the droplet is 0.88. The relaxation parameter $\tau$ is 0.1 and surface tension parameter $\kappa_s$ is 0.001. The arrows represent spatial velocities.

6. Conclusion

In this paper we proposed a lattice Boltzmann scheme for the simulation of viscous, compressible, and heat-conducting flows for nonideal fluid by introducing tensor type forces. This model recovers the complete macroscopic equations for nonideal fluids and models thermal two-phase fluid flows well.

The transport coefficients, including viscosity and thermal conductivity derived form the Chapman-Enskog expansion, were quantitatively verified in simulations of Poiseuille flow and Couette flow. The surface tension obtained by this model agrees well with Laplace’s law. The several simulations, including spontaneous phase transition and motions of bubble and droplet under gravitational force, demonstrated the applicability of this LB model to two-phase dynamics with thermal effects. Since the LB equation was solved with finite difference schemes by implementing the upwind scheme for the interfacial problems, this LB model did not encounter any numerical in-
stability when $\Delta t$ is controlled ($<\Delta x/|v_e|$).

The present paper demonstrates that the LBM is a flexible and powerful tool for modeling physical phenomena which are not easily described by macroscopic equations, and that it can be solved locally, explicitly and efficiently on parallel computers.

To compare with theoretical solutions or with experimental results, it is considered necessary to threedimensionalize this LB model. We already tried to develop three dimensional version with 21-velocity or 33velocity cubic lattice unit as Takada et al. did(9). In the three dimensional model, due to the addition of the one dimension and the increment of the number of particle velocity, the number of tensor calculated in the potential increases. As a consequence of the increase, the potential becomes stronger than two dimensional version. The large potential effect makes the three dimensional model numerically unstable. To ensure the stability, it may be necessary that the accuracy of the model is degraded. It is subject for a future study to develop a stable and high accurate three dimensional model based on this proposed LB model.

In the simulations indicated above, the liquid density is 5.767 and vapor density is 1.400, the density ratio is approximately 4.0. That is not practical for simulation of liquid-gas two-phase flows at ordinary temperatures. To simulate the two-phase flows at room temperature, the proposed LB model should stably calculate high density ratio. Recently Inamuro et al. proposed lattice Boltzmann method capable of calculating high density ratio using additional distribution function for index function$^{30,31}$.

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