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Pressure evolution lattice-Boltzmann-equation method for two-phase flow with phase change

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A lattice-Boltzmann-equation method for nonideal gases augmented by the pressure evolution equation is proposed to simulate isothermal two-phase fluid flow with phase change. The pressure evolution equation is derived by taking time derivative of the equation of state for nonideal gases. Unlike previous methods that use the equation of state to update pressure, the pressure field is evolved using the pressure evolution equation. The new approach has two advantages. First, it can avoid spurious pressure fluctuations at phase interfaces that develop owing to the pressure update by the equation of state, thus improving numerical stability of the method. Second, it permits compressibility of the fluid at phase interfaces when phase change occurs due to pressurization and depressurization. The proposed method is applied to simulate an isothermal phase change process. The numerical result is in excellent agreement with the analytical solution.

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I. INTRODUCTION

Among many successful applications of the lattice-Boltzmann-equation (LBE) methods to fluid mechanics, the LBE methods for nonideal gases or binary fluids have witnessed most significant progress in recent years [1–10]. Most of these two-phase LBE methods can be considered as diffuse interface methods [11] in that the phase interface is spread on grid points and the surface tension is transformed into a volumetric force. Generally, diffuse interface methods have some advantages over sharp interface methods because computations are much easier for three-dimensional (3D) flows in which topological change of the interfaces is complicated. They are especially useful when phase change is under consideration [12], since the speed of displacement of the interface must be explicitly computed in sharp interface methods. In addition, they are appropriate for some problems that are currently tough for sharp interface methods such as contact line dynamics and coalescence of droplets. As diffuse interface methods, the LBE methods naturally share all of these characteristics.

Recently, He, Shan, and Doolen [13] proposed an LBE formulation for nonideal gases based on the continuous discrete Boltzmann equation (DBE) using a single-relaxation-time approximation [14]. It is a promising formulation because the analysis of other schemes that incorporate intermolecular forces into LBE methods can be clearly performed in the framework of the proposed formulation. They showed that anisotropy found in other schemes is a consequence of an inappropriate intermolecular interaction. Using the formulation with some modifications. He *et al.* simulated single- and multiple-mode Rayleigh-Taylor instabilities in two dimensions [7] and three dimensions [8], and reported excellent results. Later, Zhang *et al.* [9,10] validated the surface tension term in the model and studied the effects of surface tension on two-phase Kelvin-Helmholtz instabilities.

Like most of previous LBE methods for one-component nonideal gases, the original derivation in Ref. [13] requires only a single-particle distribution function for the transport of mass and momentum. The density ρ and the velocity $\mathbf{u}$ are updated by taking moments of the particle distribution function, and the thermodynamic pressure $p^{(t)}$ is obtained from the equation of state (EOS) for nonideal gases, e.g., the van der Waals EOS. However, they have not reported any numerical simulations using the original formulation. To our knowledge, the original formulation [13] is numerically unstable due to severe pressure fluctuations at phase interfaces in which $\partial_\rho p^{(t)}$ changes its sign. In the working method [7–10], they introduced a second-particle distribution function for the transport of the order parameter or the density in particular. The DBE and LBE for the *mass* and *momentum* are then transformed into the DBE and LBE for the *pressure* and *momentum* under the assumption of incompressibility of the fluid. The resulting macroscopic equations include the continuity equation, the momentum equation, and the artificial compressibilitylike equation for the pressure. Largely due to the transformation, numerical stability is significantly improved though at the cost of solving another set of distribution function for the continuity equation. He, Chen, and Zhang [7] argued that the stability was gained due to the smaller magnitude of the external body force term after the transformation. Chen *et al.* [15] adopted the above single-particle-distribution-function LBE method for nonideal gases with the aid of a total variation diminishing scheme to simulate two-phase flow having a large density ratio.

Despite all the excellent results presented in Refs. [7–10], it should be pointed out that their working method leaves ambiguity and poses some problems of physical origin. Inconsistent temporal discretization (e.g., the explicit Euler method for the collision term and the Crank-Nicolson method for the external body force terms) reduces the order of accuracy of the scheme (see Appendix A) and omission of some body force terms in the equation for the order parameter results in spurious gradients of these terms (see Appendix B). On top of all these, the pressure in the model is not uniquely defined. The pressure in the intermolecular interaction term for nonideal gases is obtained from the EOS and is

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*Electronic address: ching-long-lin@uiowa.edu therefore the thermodynamic pressure, while the pressure updated by taking moment of the particle distribution function is the hydrodynamic pressure approximately satisfying incompressibility as in the artificial compressibility method [16]. If phase change occurs, the fluid cannot remain incompressible at phase interfaces and the effect of compressibility must be taken into account.

From different perspective, the equation for the pressure recovered from the LBE method in Refs. [7–10] can be regarded as a simplified version of the pressure evolution equation rather than the artificial compressibilitylike equation as interpreted by Refs. [7,17]. The reason why the LBE methods based on single-particle distribution function could be unstable at phase interfaces lies in evaluation of the pressure. Updating the pressure via the EOS often generates erroneous pressure fluctuations at phase interfaces due to numerical diffusion [18]. Alternatively, if the pressure is updated by the pressure evolution equation, the pressure equilibrium among fluid components is automatically maintained and the generation of spurious pressure fluctuations can be avoided [19,20]. It is speculated that the success of the LBE method in Refs. [7–10] is mainly due to the introduction of the pressure evolution equation even though it is derived for incompressible flows and appropriate only for ideal gases.

The objective of the paper is to present a different LBE method based on the pressure evolution equation for simulation of one-component two-phase fluid flow with phase change. The DBE and LBE that recover the general pressure evolution equation for nonideal gases will be derived. We will show that the artificial compressibilitylike equation found in Refs. [7–10] is a simplified version of the general pressure evolution equation and only valid for the special case of ideal gas flow in the incompressible limit. Major difficulties with this special case arise when phase change occurs. Unlike immiscible models for binary fluids [11], a model for isothermal liquid-vapor flow is supposed to predict phase change due to pressurization and depressurization. Since the pressure updated by the ideal gas pressure evolution equation only satisfies incompressibility, the pressure is decoupled from the density variation and consequently, correct phase change is hardly expected. Solving the appropriate pressure evolution equation also removes the dual meanings of the pressure.

The paper is organized as follows. In Sec. II, the discrete Boltzmann equation for a one-component two-phase fluid model by He, Shan, and Doolen [13] is reviewed to elucidate the pressure update procedure using the van der Waals EOS. In Sec. III, the pressure evolution equation for nonideal gases is derived and compared with that for ideal gases, and the corresponding DBE is given in Sec. IV. The LBE method based on the pressure evolution equation is presented in Sec. V. Section VI is devoted to testing the method by a one-dimensional isothermal phase change problem. The method is also compared with the two-phase LBE method that assumes incompressibility and utilizes the ideal gas pressure evolution equation. Concluding remarks are given in Sec. VII.

II. DISCRETE BOLTZMANN EQUATION FOR NONIDEAL GASES

The discrete Boltzmann equation for nonideal gases proposed by He, Shan, and Doolen [13] reads

$$D_t f_\alpha = \partial_t f_\alpha + e_{\alpha i}\partial_i f_\alpha = -\frac{1}{\lambda}(f_\alpha - f_\alpha^{\mathrm{eq}}) + \frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2} f_\alpha^{\mathrm{eq}}, \tag{2.1}$$

where f_α is the single-particle distribution function in the α direction of a lattice model, $e_{\alpha i}$ is the i component of the α-direction microscopic velocity, F_i is an external body force which can depend on both space and time, λ is the relaxation time due to collision, and f_α^{eq} is the equilibrium distribution function.

Equation (2.1) with the equilibrium distribution function [21]

$$f_\alpha^{\mathrm{eq}} = t_\alpha \rho\left[1 + \frac{e_{\alpha i}u_i}{c_s^2} + \frac{(e_{\alpha i}e_{\alpha j} - c_s^2\delta_{ij})u_i u_j}{2c_s^4}\right], \tag{2.2}$$

where t_α is a weighting factor, recovers the macroscopic mass and momentum equations:

$$\partial_t \rho + \partial_i(\rho u_i) = 0, \tag{2.3}$$

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = \partial_j \sigma_{ij}^{(ig)} + F_i, \tag{2.4}$$

where $\sigma_{ij}^{(ig)} = -\rho c_s^2 \delta_{ij} + \mu(\partial_j u_i + \partial_i u_j)$.

The desired form of the momentum equation for nonideal gases [22] is

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = \partial_j \sigma_{ij} + \rho g_i, \tag{2.5}$$

where ρg_i is the gravity force. The stresses σ_{ij} can be decomposed into three parts: $\sigma_{ij} = -p^{(t)}\delta_{ij} + \sigma_{ij}^{(v)} + \sigma_{ij}^{(1)}$. Here, $p^{(t)} = p^{(t)}(\rho)$ is the bulk thermodynamic pressure for the isothermal fluid and $\sigma_{ij}^{(v)}$ is the viscous stress tensor,

$$\sigma_{ij}^{(v)} = \mu(\partial_j u_i + \partial_i u_j) + \xi \partial_k u_k \delta_{ij}, \tag{2.6}$$

where μ is the molecular viscosity and $\xi = -2/3\mu$ is the bulk viscosity. The stress $\sigma_{ij}^{(1)}$ is derived from the van der Waals–Cahn-Hilliard free energy and takes the form of

$$\sigma_{ij}^{(1)} = \kappa\left[\left(\frac{1}{2}|\nabla\rho|^2 + \rho\nabla^2\rho\right)\delta_{ij} - \partial_i\rho\partial_j\rho\right]. \tag{2.7}$$

κ is related to the magnitude of the surface tension force. The van der Waals–Cahn-Hilliard free energy was originally derived to describe the near-critical behavior of mixtures, when the density gradients are small. However, it is generally considered to be valid even when the density gradients become large [23]. Equation (2.7) can be rearranged as

$$\sigma_{ij}^{(1)} = -\kappa(\rho\nabla^2\rho\delta_{ij} + T_{ij}), \tag{2.8}$$

where in two dimensions

$$[T_{ij}]=\begin{bmatrix}(\partial_x^2\rho-\partial_y^2\rho)/2 & \partial_x\rho\partial_y\rho\\ \partial_x\rho\partial_y\rho & -(\partial_x^2\rho-\partial_y^2\rho)/2\end{bmatrix}. \tag{2.9}$$

Since $\sigma_{ij}^{(ig)}\neq\sigma_{ij}$, the external force F_i is chosen to satisfy $\partial_j\sigma_{ij}^{(ig)}+F_i=\partial_j\sigma_{ij}$,

$$F_i=-\partial_j(p^{(t)}-\rho c_s^2)\delta_{ij}+\partial_j\left(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij}\right)+\rho g_i. \tag{2.10}$$

In Refs. [7,13], F_i was chosen by considering the intermolecular attraction and the effects of the exclusion volume of the molecules on the equilibrium properties of a dense gas. In either case, the final F_i's take the same form.

The macroscopic equations recovered from the DBE with the above body force F_i are

$$\partial_t\rho+\partial_i(\rho u_i)=0, \tag{2.11}$$

$$\begin{aligned}\partial_t(\rho u_i)+\partial_j(\rho u_i u_j)&=-\partial_j p^{(t)}\delta_{ij}+\partial_j\left[\mu(\partial_j u_i+\partial_i u_j)-\frac{2}{3}\mu\partial_k u_k\delta_{ij}\right]\\&\quad+\partial_j\sigma_{ij}^{(1)}+\rho g_i,\end{aligned} \tag{2.12}$$

where the molecular viscosity is given by $\mu=\rho\lambda c_s^2$. To close the system, we need an EOS. For instance, the van der Waals EOS normalized by the critical density ρ_c, the critical temperature T_c, and the reference speed of sound $c_s=\sqrt{RT}=1/\sqrt{3}$, R being the gas constant, reads

$$p^{(t)}(\rho)=\rho_c\left(\frac{\tilde{\rho}}{3-\tilde{\rho}}-\frac{3\tilde{\rho}^2}{8\tilde{T}}\right), \tag{2.13}$$

where $\tilde{\rho}=\rho/\rho_c$ and $\tilde{T}=T/T_c$. If $\tilde{T}<1$, there is a region of negative $\partial_\rho p^{(t)}$, which separates liquid and vapor phases of the fluid.

III. PRESSURE EVOLUTION EQUATION

In Refs. [19,20], the pressure evolution equation was derived for multicomponent ideal gases. In what follows, we will show the general pressure evolution equation for nonideal gases. The general evolution equation for the pressure $p^{(t)}$ is obtained by taking time derivative of the EOS and utilizing the continuity equation:

$$\partial_t p^{(t)}+\rho\partial_\rho p^{(t)}\partial_i u_i+u_i\partial_i p^{(t)}=0, \tag{3.1}$$

where $\partial_\rho p^{(t)}$ is the speed of sound that may not be constant for nonideal gases and even changes the sign at the phase interfaces. Consider a two-phase system in which liquid and vapor are in pressure equilibrium so that both pressure and velocity are constant and continuous across the phase interfaces. According to Refs. [19,20] that considered two-fluid systems, if the pressure is evolved using Eq. (3.1), the pressure at the interface remains constant and the pressure equilibrium between two phases is automatically maintained.

Assuming ideal gases with a constant speed of sound $\partial_\rho p=c_s^2$, the pressure evolution equation reduces to

$$\partial_t p^{(t)}+\rho c_s^2\partial_i u_i+u_i\partial_i p^{(t)}=0. \tag{3.2}$$

Equation (3.2) is solved in Refs. [7–10] under the assumption of $u_i\partial_i p^{(t)}\sim O(\mathrm{Ma}^3)$ (Ma, Mach number), which is equivalent to solving an equation for the hydrodynamic pressure $p^{(h)}$,

$$\partial_t p^{(h)}+\rho c_s^2\partial_i u_i=0. \tag{3.3}$$

Equation (3.3) is identified as Chorin's [16] artificial compressibilitylike equation in Refs. [10,17]. In the incompressible limit, the time derivative of the pressure becomes small and the incompressible condition is almost satisfied. This interpretation, however, poses three nontrivial problems when nonideal gases are under consideration. First, the assumption of the constant speed of sound in the derivation of Eq. (3.2) becomes invalid for nonideal gases. Second, the assumption of negligible $u_i\partial_i p^{(t)}$ in Eq. (3.2) at phase interfaces is questionable for nonideal gases. Third, use of Eq. (3.3) results in dual meanings of the pressure in the model. The pressure in the intermolecular interaction term is the thermodynamic pressure $p^{(t)}$ which is given by the EOS and is a function of the density. The pressure in Eq. (3.3) is the hydrodynamic pressure $p^{(h)}$ whose role is simply to enforce the incompressible condition of free velocity divergence and is obtained by taking moment of the particle distribution function. This inconsistency even complicates the physical meaning of the pressure in the presence of phase change. During phase change due to pressurization and depressurization, $\partial_\rho p^{(t)}$ undergoes non-negligible change in both sign and magnitude across the phase interfaces and the effects of compressibility of the fluid must be considered [24].

Equation (2.13) can be used to determine the thermodynamic pressure in the momentum equation. However, updating the pressure via the EOS often generates erroneous pressure fluctuations at the phase interfaces. According to Karni [19], "These oscillations are not the ones commonly associated with high-order schemes . . . They not only render the solutions (at times fatally) oscillatory, but also set off dispersive acoustic mechanisms which tend to further thicken the interface." Therefore, if the pressure is updated using the pressure evolution equation, the pressure equilibrium among fluid components is automatically maintained and the generation of spurious pressure fluctuations can be avoided.

IV. DISCRETE BOLTZMANN EQUATIONS FOR PRESSURE EVOLUTION MODEL

In this section, the DBEs for isothermal two-phase flow with phase change are derived according to the pressure evolution equation (3.1). The DBE (2.1) for the *mass* and *momentum* equations is transformed into that for the *pressure evolution* and *momentum* equations. He, Chen, and Zhang [7] first used the transformation to obtain the pressure evolution equation for ideal gases, viz., Eq. (3.3). They, however, interpreted the pressure evolution equation as the equation that enforces incompressibility in the artificial compressibilitylike method.

In order to perform the transformation, we define a new particle distribution function

$$g_\alpha = f_\alpha c_s^2 + (p^{(t)} - \rho c_s^2)\Gamma_\alpha(0), \tag{4.1}$$

where

$$\Gamma_\alpha(\mathbf{u}) = t_\alpha\left[1 + \frac{e_{\alpha i}u_i}{c_s^2} + \frac{(e_{\alpha i}e_{\alpha j} - c_s^2\delta_{ij})u_iu_j}{2c_s^4}\right]. \tag{4.2}$$

Taking the total derivative D_t of the new variable g_α gives

$$\begin{aligned} D_t g_\alpha &= c_s^2 D_t f_\alpha + D_t p^{(t)}\Gamma(0) - c_s^2 D_t\rho\Gamma(0) \\ &= -\frac{1}{\lambda}(g_\alpha - g_\alpha^{\mathrm{eq}}) - (e_{\alpha i} - u_i)[\partial_i(p^{(t)} - \rho c_s^2) \\ &\quad - \partial_j(\sigma_{ij}^{(1)} - \tfrac{2}{3}\mu\partial_k u_k\delta_{ij}) + \rho g_i]\Gamma(\mathbf{u}) + D_t p^{(t)}\Gamma(0) \\ &\quad - c_s^2 D_t\rho\Gamma(0), \end{aligned} \tag{4.3}$$

where the new equilibrium g_α^{eq} is

$$g_\alpha^{\mathrm{eq}} = t_\alpha\left[p^{(t)} + \rho c_s^2\left(\frac{e_{\alpha i}u_i}{c_s^2} + \frac{(e_{\alpha i}e_{\alpha j} - c_s^2\delta_{ij})u_iu_j}{2c_s^4}\right)\right]. \tag{4.4}$$

The last two terms on the right-hand side of Eq. (4.3) can be expanded through the continuity equation as follows:

$$D_t p^{(t)} = \partial_t p^{(t)} + e_{\alpha i}\partial_i p^{(t)} = -\partial_\rho p^{(t)}\partial_i\rho u_i + e_{\alpha i}\partial_i p^{(t)} \tag{4.5}$$

and

$$D_t\rho = \partial_t\rho + e_{\alpha i}\partial_i\rho = -\partial_i\rho u_i + e_{\alpha i}\partial_i\rho. \tag{4.6}$$

He, Chen, and Zhang [7] further assumed incompressible fluids, i.e., $\partial_i u_i = 0$, to reduce the above two equations to

$$D_t p^{(t)} = -\partial_\rho p^{(t)}\partial_i\rho u_i + e_{\alpha i}\partial_i p^{(t)} = (e_{\alpha i} - u_i)\partial_i p^{(t)} \tag{4.7}$$

and

$$D_t\rho = -\partial_i\rho u_i + e_{\alpha i}\partial_i\rho = (e_{\alpha i} - u_i)\partial_i\rho. \tag{4.8}$$

This eventually leads to the pressure evolution equation for ideal gases, Eq. (3.2), or the artificial compressibilitylike equation (3.3) rather than the pressure evolution equation for nonideal gases, Eq. (3.1).

Finally, Eqs. (4.5) and (4.6) are substituted into the DBE for g_α:

$$\begin{aligned} \partial_t g_\alpha + e_{\alpha i}\partial_i g_\alpha = {}& -\frac{1}{\lambda}(g_\alpha - g_\alpha^{\mathrm{eq}}) - (e_{\alpha i} - u_i)[\partial_i(p^{(t)} - \rho c_s^2) - \partial_j(\sigma_{ij}^{(1)} - \tfrac{2}{3}\mu\partial_k u_k\delta_{ij}) + \rho g_i]\Gamma(\mathbf{u}) + e_{\alpha i}\partial_i(p^{(t)} - \rho c_s^2)\Gamma(0) \\ & - (\partial_\rho p^{(t)} - c_s^2)\partial_i(\rho u_i)\Gamma(0). \end{aligned} \tag{4.9}$$

Now that the continuity equation is transformed into the pressure evolution equation, we need another distribution function for the continuity equation. The DBE for the density is simply Eq. (2.1) with the body force introduced above:

$$\partial_t f_\alpha + e_{\alpha i}\partial_i f_\alpha = -\frac{1}{\lambda}(f_\alpha - f_\alpha^{\mathrm{eq}}) - \frac{(e_{\alpha i} - u_i)[\partial_i(p^{(t)} - \rho c_s^2) - \partial_j(\sigma_{ij}^{(1)} - \frac{2}{3}\mu\partial_k u_k\delta_{ij}) + \rho g_i]}{c_s^2}\Gamma(\mathbf{u}). \tag{4.10}$$

If the terms associated with $(\sigma_{ij}^{(1)} - \frac{2}{3}\mu\partial_k u_k\delta_{ij})$ and ρg_i are omitted, spurious derivatives of these terms appear in the Chapman-Enskog expansion as shown in Appendix B.

The macroscopic equations recovered through the Chapman-Enskog expansion are

$$\partial_t\rho + \partial_i(\rho u_i) = 0, \tag{4.11}$$

$$\partial_t(\rho u_i) + \partial_j(\rho u_i u_j) = -\partial_j p^{(t)}\delta_{ij} + \partial_j\left[\mu(\partial_j u_i + \partial_i u_j) - \frac{2}{3}\mu\partial_k u_k\delta_{ij}\right] + \partial_j\sigma_{ij}^{(1)} + \rho g_i, \tag{4.12}$$

and

$$\partial_t p^{(t)} + \rho\partial_\rho p^{(t)}\partial_i u_i + u_i\partial_i p^{(t)} = 0, \tag{4.13}$$

where the molecular viscosity is given by $\mu = \rho\lambda c_s^2$. It is instructive to compare the above equations with Eqs. (2.11)–(2.13) representative of the LBE method that employs a single-particle distribution function and adopts the pressure update procedure via the EOS. The only difference between them is the pressure update procedure. The two-phase LBE method of Refs. [7–10] recovers the order parameter equation (C1) rather than the density equation (4.11) and the ideal gas pressure evolution (3.2) rather than Eq. (4.13).

V. LATTICE BOLTZMANN EQUATIONS

In order to numerically solve the DBEs, Eqs. (4.9) and (4.10), these equations are discretized along characteristics over time step δt. The LBE for f_α thus obtained is

$$f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)-f_\alpha(\mathbf{x},t)=-\int_t^{t+\delta t}\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\lambda}dt-\int_t^{t+\delta t}\frac{(e_{\alpha i}-u_i)[\partial_i(p^{(i)}-\rho c_s^2)-\partial_j(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]}{c_s^2}\Gamma(\mathbf{u})dt. \tag{5.1}$$

Note that the time integration in $[t,t+\delta t]$ is coupled with the space integration in $[\mathbf{x},\mathbf{x}+\mathbf{e}_\alpha\delta t]$. The Chapman-Enskog analysis shows that the trapezoidal rule must be used for both of the integrations in order not to introduce any spurious derivatives of the second term into the system while retaining second-order accuracy. Application of the trapezoidal rule leads to

$$\begin{aligned}f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)-f_\alpha(\mathbf{x},t)=&-\frac{1}{2}\left[\left.\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\tau}\right|_{(\mathbf{x},t)}+\left.\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\tau}\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}\right]\\&-\frac{\delta t}{2}\left[\frac{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)-\partial_j(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]}{c_s^2}\Gamma(\mathbf{u})\right]_{(\mathbf{x},t)}\\&-\frac{\delta t}{2}\left[\frac{(e_{\alpha i}-u_i)[\partial_i(p^{(i)}-\rho c_s^2)-\partial_j(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]}{c_s^2}\Gamma(\mathbf{u})\right]_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)},\end{aligned} \tag{5.2}$$

where $\tau=\lambda/\delta t$.

Likewise, the LBE for g_α is

$$\begin{aligned}g_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)-g_\alpha(\mathbf{x},t)=&-\frac{1}{2}\left[\left.\frac{g_\alpha-g_\alpha^{\mathrm{eq}}}{\tau}\right|_{(\mathbf{x},t)}+\left.\frac{g_\alpha-g_\alpha^{\mathrm{eq}}}{\tau}\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}\right]-\frac{\delta t}{2}\{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)\\&-\partial_j(\sigma_{ij}^{(1)}-\tfrac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]\Gamma(\mathbf{u})\}_{(\mathbf{x},t)}+\frac{\delta t}{2}[e_{\alpha i}\partial_i(p^{(t)}-\rho c_s^2)\Gamma(0)\\&-(\partial_\rho p^{(t)}-c_s^2)\partial_i\rho u_i\Gamma(0)]_{(\mathbf{x},t)}-\frac{\delta t}{2}\{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)\\&-\partial_j(\sigma_{ij}^{(1)}-\tfrac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]\Gamma(\mathbf{u})\}_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}+\frac{\delta t}{2}[e_{\alpha i}\partial_i(p^{(t)}-\rho c_s^2)\Gamma(0)\\&-(\partial_\rho p^{(t)}-c_s^2)\partial_i\rho u_i\Gamma(0)]_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}.\end{aligned} \tag{5.3}$$

The above LBEs are solved in the following three steps.

A. Prestreaming collision step

$$\hat{f}_\alpha(\mathbf{x},t)=f_\alpha(\mathbf{x},t)-\left.\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{2\tau}\right|_{(\mathbf{x},t)}-\frac{\delta t}{2}\left.\frac{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)-\partial_j(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]}{c_s^2}\Gamma(\mathbf{u})\right|_{(\mathbf{x},t)}, \tag{5.4}$$

$$\begin{aligned}\hat{g}_\alpha(\mathbf{x},t)=g_\alpha(\mathbf{x},t)-&\left.\frac{g_\alpha-g_\alpha^{\mathrm{eq}}}{2\tau}\right|_{(\mathbf{x},t)}-\frac{\delta t}{2}\{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)-\partial_j(\sigma_{ij}^{(j)}-\tfrac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]\Gamma(\mathbf{u})\}_{(\mathbf{x},t)}\\&+\frac{\delta t}{2}[e_{\alpha i}\partial_i(p^{(t)}-\rho c_s^2)\Gamma(0)-(\partial_\rho p^{(t)}-c_s^2)\partial_i\rho u_i\Gamma(0)]_{(\mathbf{x},t)}.\end{aligned} \tag{5.5}$$

B. Streaming step

$$\hat{f}_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)=\hat{f}_\alpha(\mathbf{x},t), \tag{5.6}$$

$$\hat{g}_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)=\hat{g}_\alpha(\mathbf{x},t). \tag{5.7}$$

C. Poststreaming collision step

$$\begin{aligned}\hat{f}_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)={}&f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)+\left.\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{2\tau}\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}\\&+\frac{\delta t}{2}\left.\frac{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)-\partial_j(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]}{c_s^2}\Gamma(\mathbf{u})\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)},\end{aligned} \tag{5.8}$$

$$\begin{aligned}\hat{g}_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)={}&g_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)+\left.\frac{g_\alpha-g_\alpha^{\mathrm{eq}}}{2\tau}\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}+\frac{\delta t}{2}\{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)\\&-\partial_j(\sigma_{ij}^{(1)}-\tfrac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]\Gamma(\mathbf{u})\}_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}-\frac{\delta t}{2}[e_{\alpha i}\partial_i(p^{(t)}-\rho c_s^2)\Gamma(0)\\&-(\partial_\rho p^{(t)}-c_s^2)\partial_i\rho u_i\Gamma(0)]_{(\mathbf{x}+\mathbf{e}_\alpha\delta,t+\delta t)}.\end{aligned} \tag{5.9}$$

The poststreaming collision step can be recast for the particle distribution functions f_α and g_α rather than $\hat{f}_\alpha$ and $\hat{g}_\alpha$ as

$$\begin{aligned}f_\alpha(\mathbf{x}+\mathbf{e}_\alpha dt,t+\delta t)={}&\hat{f}_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)-\frac{1}{2\tau+1}(\hat{f}_\alpha-f_\alpha^{\mathrm{eq}})\Big|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}\\&-\frac{\tau\delta t}{2\tau+1}\left.\frac{(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)-\partial_j(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]}{c_s^2}\Gamma(\mathbf{u})\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)},\end{aligned} \tag{5.10}$$

$$\begin{aligned}g_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)={}&\hat{g}(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)-\frac{1}{2\tau+1}(\hat{g}_\alpha-g_\alpha^{\mathrm{eq}})\Big|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}-\frac{\tau\delta t}{2\tau+1}[(e_{\alpha i}-u_i)[\partial_i(p^{(t)}-\rho c_s^2)\\&-\partial_j(\sigma_{ij}^{(1)}-\tfrac{2}{3}\mu\partial_k u_k\delta_{ij})+\rho g_i]\Gamma(\mathbf{u})]_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}+\frac{\tau\delta t}{2\tau+1}[e_{\alpha i}\partial_i(p^{(t)}-\rho c_s^2)\Gamma(0)\\&-(\partial_\rho p^{(t)}-c_s^2)\partial_i\rho u_i\Gamma(0)]_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}.\end{aligned} \tag{5.11}$$

The density, the velocity, and the pressure are calculated below after the streaming step:

$$\rho=\sum_\alpha \hat{f}_\alpha, \tag{5.12}$$

$$\rho c_s^2 u_i=\sum_\alpha \mathbf{e}_\alpha\hat{g}_\alpha+\frac{c_s^2\delta t}{2}\partial_j\left(\sigma_{ij}^{(1)}-\frac{2}{3}\mu\partial_k u_k\delta_{ij}\right)+\frac{c_s^2\delta t}{2}\rho g_i, \tag{5.13}$$

$$p^{(t)}=\sum_\alpha \hat{g}_\alpha-\frac{\delta t}{2}(\partial_\rho p^{(t)}-c_s^2)\partial_i\rho u_i, \tag{5.14}$$

where $\partial_\rho p^{(t)}$ is analytically given by the EOS and $\nu=\mu/\rho$ is the kinematic viscosity. The velocity divergence term on the right-hand side of Eq. (5.13) can be evaluated explicitly at the previous time step or implicitly using an iterative approach.

VI. ONE-DIMENSIONAL ISOTHERMAL PHASE CHANGE PROBLEM

In this section, a one-dimensional isothermal phase change problem as shown schematically in Fig. 1 is examined to compare the nonideal gas pressure evolution LBE method (NIG-PEM) described in Sec. V with the ideal gas pressure evolution LBE method (IG-PEM) that assumes incompressibility and recovers Eq. (3.2). The IG-PEM differs

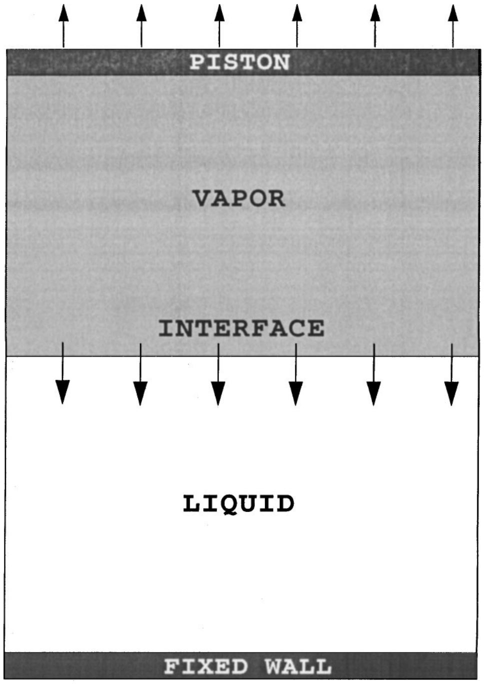

FIG. 1. Schematic representation of a one-dimensional isothermal phase-change problem.

from the two-phase LBE method of Refs. [7–10] in two aspects. In the IG-PEM, the Crank-Nicolson method is applied consistently as explained in Appendix B and the density is used as the order parameter to recover the continuity equation (2.11) as discussed in Appendix C. As the piston is withdrawn, the vapor pressure decreases to vaporize the liquid near the phase interface for thermal equilibrium. Here, we assume large thermal conductivity, and slow and isothermal phase change [12].

Two-dimensional nine-speed velocity lattice model is used [21] and computations are carried out on a periodic domain in the horizontal direction. The lower boundary is kept stationary and the upper boundary has a velocity of U in the vertical direction. All the variables are assumed to have zero normal gradient at boundaries. The central difference scheme is used to evaluate the gradient terms in the collision steps and the directional derivative of any variable ψ in the $\mathbf{e}_\alpha$ direction is discretized as

$$\mathbf{e}_\alpha \cdot \boldsymbol{\nabla} \psi(\mathbf{x}) = \frac{[\psi(\mathbf{x}+\mathbf{e}_\alpha) - \psi(\mathbf{x}-\mathbf{e}_\alpha)]}{2}. \tag{6.1}$$

Figure 2 compares the results calculated from the NIG-PEM with those of the IG-PEM. Time is measured in H/U, where H is the vertical dimension of the domain. $U=0.002$, $H=256$, $\rho_c=1$, and $\tilde{T}=0.8$ in the EOS (2.13) for which $\tilde{\rho}_l=1.871$ and $\tilde{\rho}_v=0.0657$, $\kappa=0$ in Eq. (2.7), the gravitational acceleration $g_i=0$, and $\tau=0.5$ are used in the simulation. Assuming that the bulk phase densities and the piston velocity remain constant, the speed of displacement of the interface is also constant and given as

$$U_i = \frac{\rho_l U_l - \rho_v U_v}{\rho_l - \rho_v}, \tag{6.2}$$

where ρ_l, ρ_v, U_l, and U_v are the bulk liquid density, the bulk vapor density, the liquid velocity, and the vapor velocity, respectively. The exact location of the interface is then determined from

$$y_i(t) = y_0 + U_i t. \tag{6.3}$$

It is clearly seen that the NIG-PEM predicts phase change correctly. The bulk phase densities remain constant under depressurization and phase change occurs in such a way to satisfy mass balance due to withdrawal of the piston. Also noticeable is the constant thickness of the interface region. The IG-PEM, however, is not able to allow phase change at the interface. The phase interface is stationary and mass balance is achieved by lowering the bulk phase densities in spite of the assumption of incompressibility of the fluid in the IG-PEM. The budgets of pressure evolution equations for nonideal gases and ideal gases, namely, Eqs. (3.1) and (3.2), together with velocity divergence are shown in Fig. 3 for comparison. Contrary to the ideal gas case, the nonideal gas pressure evolution equation Eq. (3.1) is approximately satisfied because of the consistent definition of the pressure. $u_i \partial_i p^{(t)}$ is non-negligible and is roughly balanced by $\rho \partial_\rho p^{(t)} \partial_i u_i$ as shown in Fig. 3(a). At the interface, $\rho \partial_\rho p^{(t)} \partial_i u_i$ for nonideal gases behaves quite differently from the ideal gas counterpart. The variation of $\rho \partial_\rho p^{(t)} \partial_i u_i$ is apparently correlated with the velocity divergence $\partial_i u_i$ term that has its maximum value near the phase interface. Thus it indicates that the compressibility of the fluid must be taken into account when phase change phenomenon is of primary interest of study.

VII. CONCLUDING REMARKS

Stability of numerical schemes for multifluid flow is sensitive to the way that the thermodynamic pressure is updated. Updating the pressure via the equation of state often generates oscillatory fluctuations in the pressure field. The pressure evolution equation is proposed by Refs. [18–20] to avoid spurious pressure fluctuations. If the pressure field is evolved by the pressure evolution equation, pressure equilibrium among fluid components is automatically maintained. In this paper, we extend this concept to one-component two-phase LBE methods and incorporate the pressure evolution equation for nonideal gases into the LBE framework. As a result, stability of the LBE methods for nonideal gases can be improved and phase change due to pressurization and depressurization can be properly simulated.

The previous incompressible lattice Boltzmann multiphase model [7–10] is identified as the ideal gas pressure evolution LBE method and is shown to be only valid for ideal gas flow in the incompressible limit. In spite of all the

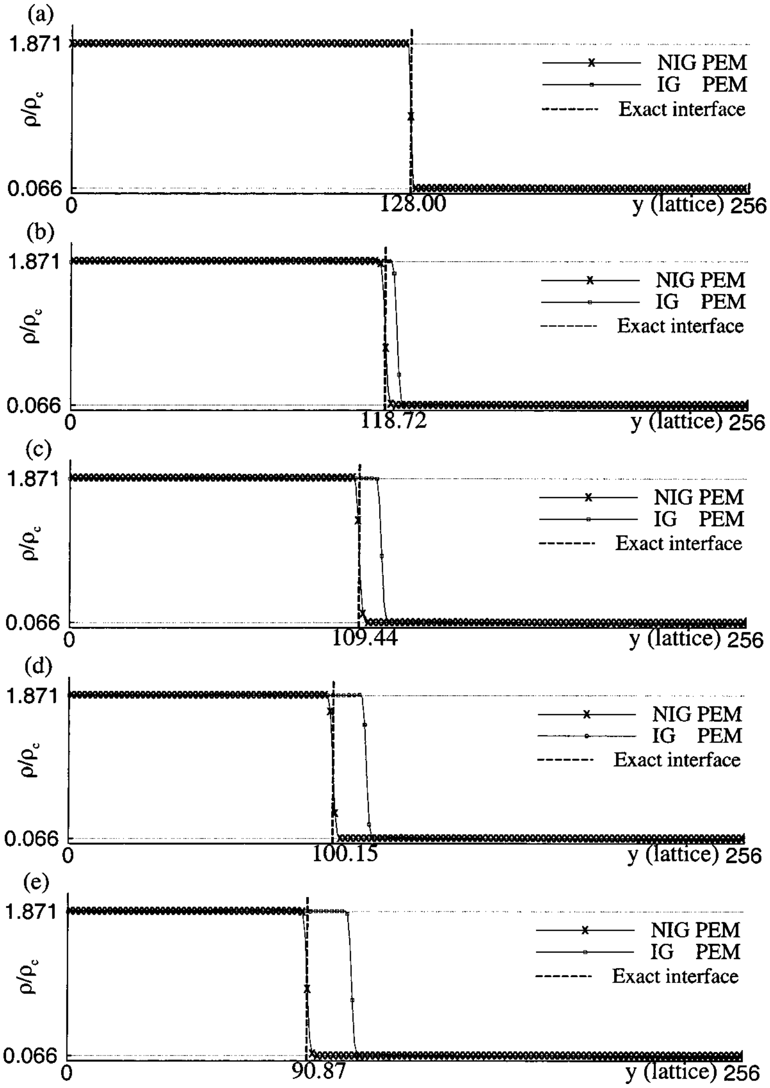

FIG. 2. Density profiles along the vertical axis at various times: (a) $t=0.0$, (b) $t=1.0$, (c) $t=2.0$, (d) $t=3.0$, and (e) $t=4.0$.

excellent results obtained by using the previous model, it is unable to predict phase change correctly, for phase change is generally involved with compressibility of the fluid at the interface region. In the present study, we propose a pressure evolution LBE method that is valid for nonideal gases and allows compressibility at the interface region in an effort to capture phase change. We use an isothermal phase change problem to study the role of the correct pressure evolution equation and the compressibility effect. Numerical experiments confirm that the nonideal gas pressure evolution LBE method predicts phase change correctly. The assumptions made in the ideal gas pressure evolution LBE method are examined by the budget analysis of the pressure evolution equation.

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APPENDIX A: INCONSISTENT TEMPORAL DISCRETIZATION

It is necessary to adopt the Crank-Nicolson temporal discretization for the collision term and the body force terms, such as the gravity force and the surface tension force, in order to achieve both second-order accuracy and unconditional stability. In most of previous literatures, however, the Crank-Nicolson discretization of the body force terms is used in conjunction with the explicit Euler discretization of the collision term. This leads to spurious gradients of those body force terms in the recovered macroscopic equations as shown below.

The discrete Boltzmann equation with the body force F_i generally expressed in Eq. (2.1) can be consistently discretized as

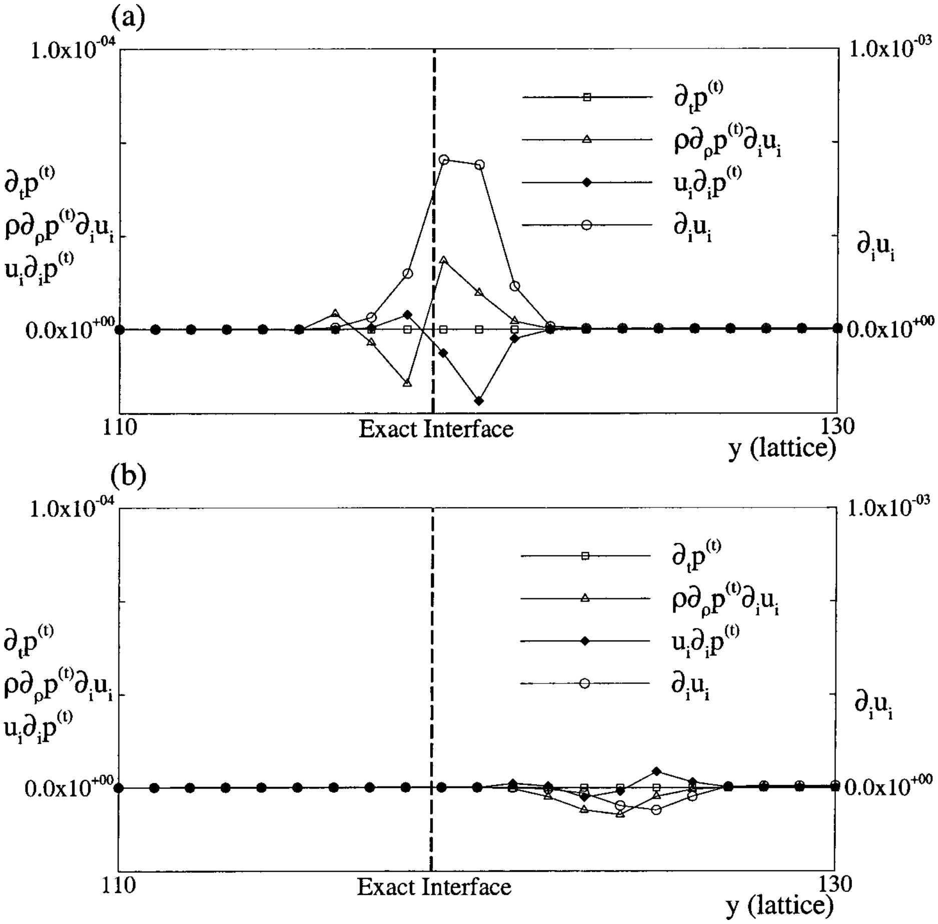

FIG. 3. Distributions of each term in the pressure evolution equation along the vertical axis at $t=1.0$: (a) NIG-PEM and (b) IG-PEM.

$$f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)-f_\alpha(\mathbf{x},t)=-\frac{1}{2}\left[\left.\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\tau}\right|_{(\mathbf{x},t)}+\left.\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\tau}\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}\right]+\frac{\delta t}{2}\left[\left.\frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2}f_\alpha^{\mathrm{eq}}\right|_{(\mathbf{x},t)}+\left.\frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2}f_\alpha^{\mathrm{eq}}\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}\right], \tag{A1}$$

where $\tau=\lambda/\delta t=\nu/(c_s^2\delta t)$. The Chapman-Enskog expansion starts from Taylor-series expansion around the point at which the collision term is defined [25], i.e., around $(\mathbf{x}+1/2\mathbf{e}_\alpha\delta t,t+1/2\delta t)$ in this case. Expansion of Eq. (A2) yields

$$\delta t\left[\frac{\partial}{\partial t}+e_{\alpha i}\partial_i\right]f_\alpha=-\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\tau}+\delta t\frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2}f_\alpha^{\mathrm{eq}}+\text{higher-order terms}. \tag{A2}$$

Mixed discretization of Eq. (2.1) as was done by Ref. [7] results in

$$f_\alpha(\mathbf{x}+\mathbf{e}_\alpha dt,t+\delta t)-f_\alpha(\mathbf{x},t)=-\left.\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\tau}\right|_{(\mathbf{x},t)}+\frac{\delta t}{2}\left[\left.\frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2}f_\alpha^{\mathrm{eq}}\right|_{(\mathbf{x},t)}+\left.\frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2}f_\alpha^{\mathrm{eq}}\right|_{(\mathbf{x}+\mathbf{e}_\alpha\delta t,t+\delta t)}\right], \tag{A3}$$

with modified τ being $\tau=\lambda/\delta t=\nu/(c_s^2\delta t)+\frac{1}{2}$. Taylor-series expansion of Eq. (A4) around $(\mathbf{x},t)$ gives

$$\delta t\left[\frac{\partial}{\partial t}+e_{\alpha i}\partial_i\right]f_\alpha+\frac{\delta t^2}{2}\left[\frac{\partial}{\partial t}+e_{\alpha i}\partial_i\right]^2f_\alpha=-\frac{f_\alpha-f_\alpha^{\mathrm{eq}}}{\tau}+\delta t\frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2}f_\alpha^{\mathrm{eq}}+\frac{\delta t^2}{2}\left[\frac{\partial}{\partial t}+e_{\alpha i}\partial_i\right]^2\frac{F_i(e_{\alpha i}-u_i)}{\rho c_s^2}f_\alpha^{\mathrm{eq}}+\text{higher-order terms}. \tag{A4}$$

Two terms which are absent in Eq. (A2) now appear. The second term on the left-hand side affects the physical viscosity that can be offset by modifying the relaxation parameter [26], but the last term on the right-hand side cannot be canceled out and remains as a second-order error term.

APPENDIX B: EFFECTS OF DROPPING BODY FORCE TERMS IN THE EQUATION FOR THE ORDER PARAMETER

He *et al.* [7,8] and Zhang *et al.* [9,10] dropped the gravity force and the surface tension force in the DBE that governs the evolution of the order parameter ϕ. Take $\phi=\rho$ (density). Equation (4.10) without these force terms is written as

$$\partial_t f_\alpha + e_{\alpha i}\partial_i f_\alpha = -\frac{1}{\lambda}(f_\alpha - f_\alpha^{\mathrm{eq}}) - \frac{(e_{\alpha i}-u_i)\partial_i(p^{(t)}-\rho c_s^2)}{c_s^2}\Gamma(\mathbf{u}). \tag{B1}$$

Assuming that the Crank-Nicolson method is applied for both the collision term and the body force terms, the macroscopic equation recovered from the Chapman-Enskog expansion takes the form of

$$\partial_t\rho + \partial_i(\rho u_i) = \partial_i\lambda\left[\partial_j\left(\sigma_{ij}^{(1)} - \frac{2}{3}\mu\partial_k u_k\delta_{ij}\right) - \rho g_i\right]. \tag{B2}$$

Note that the right-hand side of the continuity equation is not zero. The spurious gradients of the terms dropped from Eq. (4.10) are proportional to the relaxation parameter λ.

APPENDIX C: EFFECTS OF USING EQ. (4.10) AS THE EQUATION FOR THE ORDER PARAMETER

He *et al.* [7,8] and Zhang *et al.* [9,10] used a variant of Eq. (4.10) for the order parameter ϕ that represents physical properties such as the density and the viscosity. Assuming that all the body forces are retained and the Crank-Nicolson scheme is consistently applied for both the collision term and the body force terms, the macroscopic equation recovered from the Chapman-Enskog expansion takes the form of

$$\partial_t\phi + \partial_i(\phi u_i) = \partial_i\lambda\left[\partial_i p^{(t)} - \frac{\phi}{\rho}\partial_i p^{(t)}\right]. \tag{C1}$$

The terms on the right-hand side are again the error terms proportional to the relaxation parameter λ. Zhang, He, and Chen [9] interpreted Eq. (C1) as a level-set-like equation but since ϕ is not a distant function in this case, this interpretation is not appropriate.

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