RAPID COMMUNICATIONS

PHYSICAL REVIEW E **68**, 035302(R) (2003)

Discrete velocity and lattice Boltzmann models for binary mixtures of nonideal fluids

Zhaoli Guo and T. S. Zhao
Department of Mechanical Engineering, The Hong Kong University of Science & Technology, Kowloon, Hong Kong

(Received 25 March 2003; published 17 September 2003)

In this paper, a discrete velocity model and a lattice Boltzmann model are proposed for binary mixtures of nonideal fluids based on the Enskog theory. The velocity space of the Enskog equation for each component is first discretized by applying a Gaussian quadrature, resulting in a discrete velocity model that can be solved by suitable numerical schemes. A lattice Boltzmann model is then derived from the discrete velocity model with a slightly modified equilibrium. The hydrodynamics of each model are also derived through the Chapmann-Enskog procedure.

DOI: 10.1103/PhysRevE.68.035302 PACS number(s): 47.11.+j, 05.20.Dd, 47.10.+g

Modeling complex systems at microscopic and mesoscopic levels is becoming a promising and viable approach in related areas. The lattice Boltzmann method (LBM) [1] is just such a method for fluid systems. A distinctive feature of LBM is that interparticle interactions can be easily incorporated into the method, so that some complex fluid behaviors, which may be rather difficult, if not impossible, to be simulated by conventional numerical methods, can be simulated efficiently by LBM. For example, in systems involving interfaces and phase change, the interfaces between different components/phases are very difficult to track by conventional techniques due to the complex geometry and possible phase change. On the other hand, it is well understood that macroscopic interfaces and phase changes are thermodynamic results of microscopic interactions between molecules, therefore, once the microscopic interactions are modeled appropriately at the microscopic or mesoscopic level, the hydrodynamic behaviors of the system will appear naturally. This is in fact what LBM and some other discrete kinetic models have done in modeling such systems [1].

Several lattice Boltzmann models and kinetic models have been proposed for multicomponent and multiphase systems [2–10]. These models are built on different physical pictures and each takes a different appearance. However, they can all be viewed as special discretizations of certain kinetic equations with certain approximations [2–5], and it is helpful to understand the advantages and disadvantages of the models from the kinetic theory point of view. Furthermore, some studies [2–5] indicate that physically consistent models can be directly derived from certain kinetic equations using some standard discretization procedures.

In this paper, we aim to develop a discrete kinetic model and a lattice Boltzmann model for binary mixtures of nonideal fluids. Unlike other previously proposed heuristic models for such systems [6,7], which were based on fictitious ‘‘intermolecular interactions’’ or *ad hoc* ‘‘free energies,’’ the present models are based on a kinetic theory for dense mixtures. It is noted that a lattice Boltzmann model for mixtures of ideal fluids has recently been proposed based on the Boltzmann equation for ideal mixtures [4].

The kinetic theory for single-component nonideal fluids was first proposed by Enskog [11], and was later generalized for binary mixtures of hard spheres by Thorne [11] and further extended to multicomponent mixtures by Tham and Gubbins [12]. Formerly, it was believed that the Enskog theory, now usually referred to as standard Enskog theory (SET), was incompatible with the linear irreversible thermodynamics (LIT) for mixtures [13], and a revised version of SET, the so-called revised Enskog theory, was proposed to fix this problem [14]. However, very recently it was shown that the SET is actually compatible with LIT [15]. Therefore, the SET can serve as a basis for developing discrete kinetic models for nonideal mixtures.

We start from the Enskog equations for a binary mixture of components 0 and 1 [15]:

$$(D_a+\mathbf{g}_a\cdot\nabla_{\mathbf{v}_a})f_a(\mathbf{x},\mathbf{v}_a,t)=\sum_b J_{ab}, \quad a=0,1, \tag{1}$$

where $D_a=\partial_t+\mathbf{v}_a\cdot\nabla$, $f_a(\mathbf{x},\mathbf{v}_a,t)$ is the single-particle distribution function for component a in the phase space $(\mathbf{x},\mathbf{v}_a)$, $\mathbf{v}_a$ is the particle velocity of sphere a with diameter σ_a and mass m_a. $\mathbf{g}_a$ is the acceleration due to an external force acting on the particle a. The collision operators between two particles of the same or different species are given by

$$\begin{aligned}J_{ab}=\int d\boldsymbol{\mu}_b[&\chi_{ab}(\mathbf{x}+y_{ab}\mathbf{k})f_b(\mathbf{x}+\sigma_{ab}\mathbf{k},\mathbf{v}_b')f_s(\mathbf{x},\mathbf{v}_a')\\&-\chi_{ab}(\mathbf{x}-y_{ab}\mathbf{k})f_b(\mathbf{x}-\sigma_{ab}\mathbf{k},\mathbf{v}_b)f_s(\mathbf{x},\mathbf{v}_a)],\end{aligned} \tag{2}$$

where $\chi_{ab}=\chi_{ab}(n_a,n_b)$ is the radial distribution function (RDF) of two hard spheres (one of component a and the other of component b) at contact, which is evaluated at a point located between the centers of the colliding particles, i.e., $y_{ab}=\sigma_{ab}/2$ with $\sigma_{ab}=(\sigma_a+\sigma_b)/2$. In Eq. (2), $\mathbf{k}$ is the unit vector directed from particle b to particle a along the line of centers of the two colliding particles. $\mathbf{v}$ and $\mathbf{v}'$ are the molecular velocities before and after the collision, respectively.

The number density of each component and the velocity of the mixture are defined by the moments of the distribution functions:

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

where $\rho=\Sigma_a m_a n_a$ is the density of the mixture.

If we expand f_a and χ_{ab} in a Taylor series up to first order in gradients about $\mathbf{x}$, use the Bhatnager-Grass-Krook (BGK) approximation [16], and assume the mixture to be isothermal and incompressible, we have [17]

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$$D_a f_a(\mathbf{x},\mathbf{v}_a,t) = -\lambda_a^{-1}[f_a - f_a^{(eq)}] + J'_a + G_a, \tag{4}$$

where

$$G_a = f_a^{(eq)}(\mathbf{v}_a - \mathbf{u})\cdot\mathbf{g}_a/\theta_a, \tag{5}$$

$$J'_a = -f_a^{(eq)}(\mathbf{v}_a - \mathbf{u})\cdot\mathbf{K}_a, \tag{6}$$

with $\mathbf{K}_a = \Sigma_b b_{ab}\rho_b\chi_{ab}\boldsymbol{\nabla}\ln(\rho_b^2\chi_{ab})$, and $b_{ab} = V_{ab}/m_b$ is the virial coefficient with $V_{ab} = 2\pi\sigma_{ab}^3/3$ in three dimensions (3D) or $\pi\sigma_{ab}^2/4$ in 2D. $f_a^{(eq)}$ is the Maxwellian local equilibrium distribution function and is given by [15]

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

with D being the dimension of the $\mathbf{v}_a$ moment space, $\theta_a = k_B T/m_a$ is the normalized temperature, and k_B is the Boltzmann constant. In what follows we assume that the two components are in local equilibrium, implying that the local equilibrium velocities of both components are equal to the local barycentric velocity of the mixture, i.e., $\mathbf{u}_0^{(eq)} = \mathbf{u}_1^{(eq)} = \mathbf{u}$.

Some remarks should be made on the relaxation time λ_a. As in the BGK models for ideal fluids [10], the local momentum conservation in the ideal fluid limit requires $\lambda_0 = \lambda_1 \equiv \lambda$. It is noted that here λ is not a constant, but a variable that may depend on the number density of each component [10].

A discrete velocity model can be derived from Eq. (4) by projecting the velocity space onto a finite set of discrete velocities. Here we follow the procedure proposed by He and Luo [18]. First, we construct an equilibrium distribution by truncating the Taylor series of $f_a^{(eq)}$ given by Eq. (7) up to second order in $\mathbf{u}$:

$$f_a^{(eq)} = \frac{n_a}{(2\pi\theta_a)^{D/2}}\exp\left(-\frac{\mathbf{v}_a^2}{2\theta_a}\right)\left[1 + \frac{\mathbf{v}_a\cdot\mathbf{u}}{\theta_a} + \frac{(\mathbf{v}_a\cdot\mathbf{u})^2}{2\theta_a^2} - \frac{\mathbf{u}^2}{2\theta_a}\right]. \tag{8}$$

We then project the velocity space onto a finite set of discrete velocities $\mathbf{e}_{ai}$ such that the numerical quadrature

$$\int \mathbf{v}_a^k f_a^{(eq)}(\mathbf{x},\mathbf{v}_a,t)\,d\mathbf{v}_a = \sum_i W_{ai}\mathbf{e}_{ai}^k f_a^{(eq)}(\mathbf{x},\mathbf{e}_{ai},t) \tag{9}$$

holds exactly for $0 \leqslant k \leqslant 3$. A natural choice for the evaluation of the integral is the Gaussian quadrature with weight function $\exp(-\mathbf{v}_a^2/2\theta_a)$. In what follows, we shall restrict ourselves to a two-dimensional nine-velocity model [19] for the sake of simplicity without losing generality. In this case, the Gaussian quadrature yields the following discrete velocities: $\mathbf{e}_{a0} = \mathbf{0}$, $\mathbf{e}_{ai} = \sqrt{3\theta_a}\{\cos[(i-1)\pi/2],\sin[(i-1)\pi/2]\}$ for $i = 1$–4, and $\mathbf{e}_{ai} = \sqrt{6\theta_a}\{\cos[(i-5)\pi/2],\sin[(i-5)\pi/2]\}$ for $i = 5$–8; the weights are given by $W_{ai} = 2\pi\theta_a\exp[\mathbf{e}_{ai}^2/(2\theta_a)]\omega_i$ with $\omega_0 = 4/9$, $\omega_i = 1/9$ for $i = 1$–4, and $\omega_i = 1/36$ for $i = 5$–8.

Once the discrete velocities $\mathbf{e}_{ai}$ and the weights W_{ai} are determined, we arrive at our first point of this paper: a discrete velocity model for binary nonideal mixtures can be defined from Eq. (4),

$$D_{ai}f_{ai}(\mathbf{x},t) = -\lambda^{-1}[f_{ai} - f_{ai}^{(eq)}] + J'_{ai} + G_{ai}, \tag{10}$$

where $D_{ai} = \partial_t + \mathbf{e}_{ai}\cdot\boldsymbol{\nabla}$, $f_{ai}(\mathbf{x},t) = W_{ai}f_a(\mathbf{x},\mathbf{e}_{ai},t)$, and

$$f_{ai}^{(eq)} = \omega_i n_a\left[1 + \frac{\mathbf{e}_{ai}\cdot\mathbf{u}}{\theta_a} + \frac{(\mathbf{e}_{ai}\cdot\mathbf{u})^2}{2\theta_a^2} - \frac{\mathbf{u}^2}{2\theta_a}\right], \tag{11}$$

$$J'_{ai} = -f_{ai}^{(eq)}(\mathbf{e}_{ai} - \mathbf{u})\cdot\mathbf{K}_a, \tag{12}$$

$$G_{ai} = f_{ai}^{(eq)}(\mathbf{e}_{ai} - \mathbf{u})\cdot\mathbf{g}_a/\theta_a. \tag{13}$$

The number density of each component and the velocity of the mixture are consequently defined as

$$n_a = \sum_i f_{ai}, \quad \rho\mathbf{u} = \sum_a m_a\sum_i \mathbf{e}_{ai}f_{ai}. \tag{14}$$

From the above definitions, it is easy to calculate the following moments:

$$\sum_i f_{ai}^{(eq)} = n_a, \quad \sum_i \mathbf{e}_{ai}f_{ai}^{(eq)} = n_a\mathbf{u}, \tag{15a}$$

$$\sum_i e_{ai\alpha}e_{ai\beta}f_{ai}^{(eq)} = \theta_a n_a\delta_{\alpha\beta} + n_a u_\alpha u_\beta, \tag{15b}$$

$$\sum_i J'_{ai} = \sum_i G_{ai} = 0, \tag{15c}$$

$$\sum_i \mathbf{e}_{ai}J'_{ai} = -n_a\theta_a\mathbf{K}_a, \quad \sum_i \mathbf{e}_{ai}G_{ai} = n_a\mathbf{g}_a. \tag{15d}$$

Through the Chapman-Enskog procedure and with the aid of Eq. (15), we can derive the mass conservation equation of component a and the hydrodynamic equations of the mixture from the discrete velocity model (10):

$$\partial_t\rho_a + \boldsymbol{\nabla}\cdot(\rho_a\mathbf{u}) = -\boldsymbol{\nabla}\cdot\mathbf{j}_a, \tag{16}$$

$$\partial_t\rho + \boldsymbol{\nabla}\cdot(\rho\mathbf{u}) = 0, \tag{17}$$

$$\partial_t(\rho\mathbf{u}) + \boldsymbol{\nabla}\cdot(\rho\mathbf{u}\mathbf{u}) = -\boldsymbol{\nabla}p + \boldsymbol{\nabla}\cdot[\rho\nu(\boldsymbol{\nabla}\mathbf{u} + (\boldsymbol{\nabla}\mathbf{u})^T)] + \sum_a \rho_a\mathbf{g}_a, \tag{18}$$

where $\mathbf{j}_a = m_a\Sigma_i(\mathbf{e}_{ai} - \mathbf{u})f_{ai}$ is the mass flux of component a, ν is the shear viscosity given by $\nu = n\lambda k_B T/\rho$; $n = n_0 + n_1$ is the total number density; $p = p_0 + p_1$ is the total pressure, and

$$p_a = \theta_a\rho_a(1 + b_{aa}\rho_a\chi_{aa} + b_{a\bar{a}}\rho_{\bar{a}}\chi_{a\bar{a}}), \quad a = 0,1, \tag{19}$$

where $\bar{a} = 1 - a$. Obviously, the pressure of the mixture satisfies a nonideal fluid equation of state. Therefore, phase transition of the mixture can be simulated using the present model by adjusting b_{ab} and χ_{ab}. In the single-component region, p reduces to the previous result for nonideal fluids. It is also noted that the viscosities of both components can take different values, although $\lambda_0=\lambda_1=\lambda$.

We now discuss the diffusion in the mixture. Equation (16) can be rewritten as

$$\rho(\partial_t X_a+\mathbf{u}\cdot\nabla X_a)=-\nabla\cdot\mathbf{j}_a, \tag{20}$$

where $X_a=\rho_a/\rho$ is the mass fraction of component a. The mass flux $\mathbf{j}_a$ can be evaluated by means of the Chapman-Enskog technique at the second order [11]. After some algebra, we obtain that

$$\mathbf{j}_a=-\lambda n k_B T\mathbf{d}_a, \tag{21}$$

where $\mathbf{d}_a$ is the diffusion force defined by [17]

$$\mathbf{d}_a=\frac{\rho_a}{n\rho k_B T}\left[\rho_{\bar{a}}\Delta\mathbf{g}_a-\nabla p+\frac{\rho}{m_a}\sum_b\frac{\partial\mu_a}{\partial n_b}\nabla n_b\right], \tag{22}$$

where $\Delta\mathbf{g}_a=\mathbf{g}_{\bar{a}}-\mathbf{g}_a$, μ_a is the chemical potential of species a and satisfies $\partial\mu_a/\partial n_b=(k_B T/n_a)E_{ab}$, with

$$E_{ab}=\delta_{ab}+2b_{ab}\rho_a\chi_{ab}+n_a\sum_c b_{ac}\rho_c\frac{\partial\chi_{ac}}{\partial n_b}. \tag{23}$$

The diffusion force $\mathbf{d}_a$ given by Eq. (22) is consistent with the phenomenological one as suggested in Ref. [15]. Furthermore, under the condition of no external forces and uniform pressure ($\mathbf{g}_a=\mathbf{g}_b=\nabla p=0$), the diffusion force reduces to [17]

$$\mathbf{d}_a=\frac{\rho^2}{m_a m_{\bar{a}} n^2}\frac{L_{\bar{a}}E_{aa}-L_a E_{a\bar{a}}}{L_{\bar{a}}x_{\bar{a}}+L_a x_a}\nabla X_a, \tag{24}$$

where $L_a=E_{\bar{a}\bar{a}}+E_{aa}$ and $x_a=n_a/n$. Therefore, under this condition, Eq. (20) reduces to

$$\rho(\partial_t X_a+\mathbf{u}\cdot\nabla X_a)=\nabla\cdot(\rho\mathcal{D}_a\nabla X_a), \tag{25}$$

where the mutual diffusivity $\mathcal{D}_a$ is given by

$$\mathcal{D}_a=\frac{\lambda\rho k_B T}{m_a m_b n}\frac{L_{\bar{a}}E_{aa}-L_a E_{a\bar{a}}}{L_{\bar{a}}x_{\bar{a}}+L_a x_a}. \tag{26}$$

Note that $\mathcal{D}_a$ can be either positive or negative, depending on the number density, the diameter ratio, and concentrations of the components of the mixture. Therefore, the proposed discrete velocity model can be used to simulate both miscible and immiscible binary mixtures.

To solve the discrete velocity equation (10) numerically, the space and time should be discretized using appropriate numerical schemes. However, one cannot expect to construct a lattice Boltzmann model directly from the discrete velocity model on a uniform lattice as usually done for single-component fluid, except for the case of $m_0=m_1$. This is because as $m_0\neq m_1$, we have $\mathbf{e}_{0i}\neq\mathbf{e}_{1i}$ for $i\neq 0$, which indicates that the configure spaces for the two components cannot be discretized on a single uniform lattice.

An alternative way to derive a lattice Boltzmann model from the discrete velocity model is to modify the equilibrium distribution function of each component such that the constraints given by Eq. (15) still hold. One such choice is to take

$$f_{ai}^{(eq)}=\begin{cases}\omega_i n_a\left[s_a+\dfrac{\mathbf{e}_i\cdot\mathbf{u}}{\theta}+\dfrac{(\mathbf{e}_i\cdot\mathbf{u})^2}{2\theta^2}-\dfrac{\mathbf{u}^2}{2\theta}\right], & i\neq 0,\\[2ex] \omega_0 n_a\left(\dfrac{1-s_a}{\omega_0}+s_a-\dfrac{\mathbf{u}^2}{2\theta}\right), & i=0,\end{cases}$$

where $s_a=\theta_a/\theta$, and θ is a reference normalized temperature of the mixture; $\mathbf{e}_i$ is redefined by $\mathbf{e}_0=\mathbf{0}$, $\mathbf{e}_i=\sqrt{3\theta}\{\cos[(i-1)\pi/2],\sin[(i-1)\pi/2]\}$ for $i=1-4$, and $\mathbf{e}_i=\sqrt{6\theta}\{\cos[(i-5)\pi/2],\sin[(5-1)\pi/2]\}$ for $i=5$–8.

Note that θ and $\mathbf{e}_i$ become identical for each component now, therefore the configurational spaces for both components can be discretized on a uniform lattice, which gives that $\theta=c^2/3$ with $c=\delta_x/\delta_t$, where δ_x is the lattice spacing and δ_t is the time increment. Now, we arrive at the second point of this paper: a lattice Boltzmann equation (LBE) can be obtained by integrating the discrete velocity equation (10) using the trapezoidal rule:

$$h_{ai}(\mathbf{x}+\mathbf{e}_i\delta_t,t+\delta_t)-h_{ai}(\mathbf{x},t)=\Omega_{ai}+F_{ai}, \tag{27}$$

where $h_{ai}=f_{ai}+(f_{ai}-f_{ai}^{(eq)})/(2\tau-1)-(J'_{ai}+G_{ai})\delta_t/2$, $\Omega_{ai}=-(h_{ai}-f_{ai}^{(eq)})/\tau$, $\tau=\lambda/\delta_t+0.5$, and $F_{ai}=\delta_t(1-0.5/\tau)(J'_{ai}+G_{ai})$. The number density of each component is defined by $n_a=\Sigma_i h_{ai}$, and the velocity of the mixture is defined by

$$\rho\mathbf{u}=\sum_a m_a\sum_i\mathbf{e}_i h_{ai}+\frac{\delta_t}{2}\sum_a\rho_a(\mathbf{g}_a-\theta_a\mathbf{K}_a). \tag{28}$$

Again, through the Chapman-Enskog procedure we can derive the conservation equations for each component and the mixture from the present LBE (27) [17]. These equations are the same as those derived from the above discrete velocity model, except that λ is replaced by $(\tau-0.5)\delta_t$ in the expressions of ν and $\mathcal{D}_a$ due to discrete effect. Therefore, as the discrete velocity model, the present LBE can also be used to simulate both miscible and immiscible binary mixtures.

In practical applications, the RDFs χ_{ab} must be specified in advance. There are several different methods to determine these RDFs. For instance, in the van den Waals one (vdW-1) fluid approximation [20], the mixture is treated as an effective single-component fluid, and all the RDFs share the same expression as that of the effective fluid, i.e., $\chi_{ab}=g(\sigma_X)$, where g is the RDF of the effective fluid, and σ_X is the effective diameter defined by $\sigma_X^D=x_0^2\sigma_0^D+2x_0x_1L_{01}\sigma_{01}^D+x_1^2\sigma_1^D$, with L_{01} being a free interaction parameter. Therefore, once the RDF of the single fluid is specified, the RDFs for the mixture are fully determined.

Using the vdW-1 approximation and the Carnahan-Starling RDF [21], $g=(1-\eta/2)/(1-\eta)^3$, where $\eta=nV_X$ is the packing factor, we applied the present LBE to a binary mixture consisting of a component with $m_0=2.0$ and another with $m_1=1.0$ on a two-dimensional 128×128 lattice with periodic boundaries. The system was initialized as $\langle n_0\rangle$

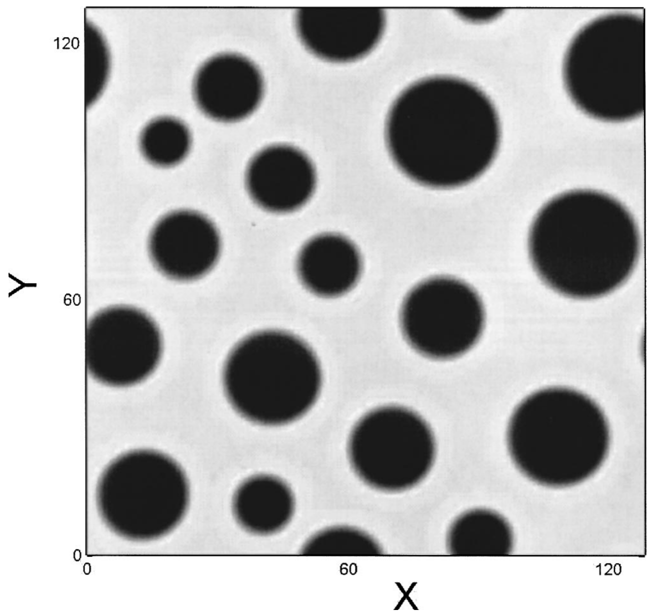

FIG. 1. Density distribution of the binary mixture at $t=10\,000$ (minimum in white and maximum in black).

$=0.3$ and $\langle n_1\rangle=0.7$ with a small random perturbation, and we set $V_0=0.025$, $V_1/V_0=0.5$. As L_{01} is large enough, the mixture will separate into two immiscible fluids. For example, as $L_{01}=6.0$, small droplets of component 0 appeared in the random mixture and merged into larger ones as time evolved. At a later stage, component 0 is seen to have completely separated from component 1 and formed into circular drops. Figure 1 shows the density distribution of the mixture at $t=10\,000$. The Laplace law $\Delta P=\sigma/R$, where ΔP is the pressure difference between the inside and the out side a circular bubble of radius R, was also verified. Initially, a circular bubble of component 0 with $m_0=1.0$ and $n_0=1.1$ was set at the center of the lattice, and the domain outside the bubble was filled with component 1 with $m_1=1.0$ and $n_0=1.0$. As the system reached its equilibrium, a bubble in circular shape formed and the pressure difference and the radius of the bubble were measured. The measurements are plotted in Fig. 2. It is seen that the Laplace law is approximately satisfied.

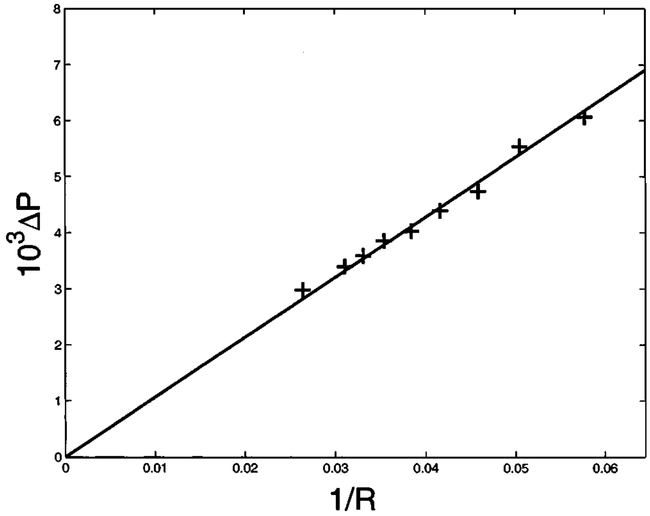

FIG. 2. Test of the Laplace law with $L_{01}=4.5$.

In summary, starting from the SET, we have constructed a discrete velocity model and a lattice Boltzmann model for mixtures of nonideal fluids. The hydrodynamic equations for the mixture and the diffusion equation are derived from both models through the Chapman-Enskog procedure. Both models can be used to simulate phase change or mixing/separating behavior of nonideal fluids. They are directly derived from the kinetic theory, and therefore have a sound physics.

Z.G. sincerely thanks Dr. LS. Luo for his great help and sharing Ref. [4] before its publication. He also thanks Dr. Y.H. Qian for his encouragements. This work was supported by a RGC grant of Hong Kong (Grant No. HKUST6193/01E).

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