

Rarefied gas flow simulations with TMAC in the slip and the transition flow regime using the lattice Boltzmann method†

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Abstract

The lattice Boltzmann (LB) method has been used to simulate rarefied gas flows in micro-systems as an alternative tool, and shown its application possibility. For the rarefied gas flows, the surface roughness plays an important role for the slip phenomenon at the wall. If the wall surface is sufficiently rough, the reflection of the molecules will be diffuse and the tangential momentum accommodation coefficient (TMAC) is equal to unity. However, it has been known that the reflections are not always fully diffuse. In this study, rarefied gas flows are simulated in the slip and the transition flow regime including the effect of the TMAC. For the simulations, new non-fully diffuse wall boundary treatments of the LB method are proposed. The results of 2D and 3D simulations are in excellent agreement with the analytical solutions for the slip flow regime. The solutions of the linearized Boltzmann equation and DSMC for the transition flow regime are compared with those of high order LB method with present boundary conditions, and they are in excellent agreement. The tangential momentum accommodation coefficient effect is also investigated.

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Keywords: Lattice Boltzmann method; Micro gas-flow; Slip and transition regime; Tangential momentum accommodation coefficient (TMAC)

1. Introduction

The lattice Boltzmann (LB) method has been recently used to simulate some rarefied gas flows in microsystem [1-5]. The rarefaction effect can be characterized by the Knudsen number *Kn*, which is the ratio of the mean free path to the characteristic length. Schaaf and Chambre [6] classified different flow regimes based on Kn . For $Kn \leq 0.01$, the fluid can be considered as a continuum, while for $Kn \geq 10$ it is considered a freemolecular flow. Between the two limits with $0.01 \leq Kn \leq 10$, which is typical of gas flows in microsystems, the flow is further classified into slip flow for $0.01 \leq Kn \leq 0.1$ and transition flow for $0.1 \leq Kn \leq 10$. For *Kn* greater than 0.01, the slip at the solid wall becomes an important flow feature. As the rarefaction effect becomes significant, the pressure drop, shear stress, heat flux, and mass flow rate cannot be properly predicted from the model based on the continuum hypothesis. Unlike conventional numerical schemes which solve the macroscopic variables directly, such as velocity and pressure, the tangential momentum accommodation coefficient (TMAC), σ , LB method is based on the microscopic kinetic equation for the particle distribution function. Because the LB method is a particle-based method, such as the direct simulation of Monte Carlo (DSMC) method [7], it is applicable to a slip flow. Most

importantly, because the LB method deals with particle distribution functions, it is more computationally efficient than the DSMC method.

In the previous slip flow simulations using the LB method, various boundary treatments were applied to obtain the slip velocity at a wall. Among them, bounce-back and specular bounce-back schemes have been widely used. Nie et al. [1] used bounce-back boundary condition for a stationary wall. In the bounce-back scheme, the particle distribution function, which streams to a wall node, scatters back to the node it comes from. However, it is known that it gives less degree of slip at a given *Kn* [4]. To enhance the slip effect, Succi [2] introduced the specular bounce-back scheme. It is a mix of bounce-back and specular reflections. Lee and Lin [4] used the equilibrium distribution function as a boundary condition. The boundary schemes of those investigations were restricted to fully diffuse flat walls. If the wall surface is sufficiently rough, the reflection of the molecules will be diffuse and the is equal to unity, which can be defined for tangential momentum exchange of gas molecules with surfaces, i.e. $\sigma = (\tau_f - \tau_f)$ τ_r)/(τ_i - τ_w), where τ_i and τ_r are the tangential momentum of incoming and reflected molecules, and τ_w is the tangential momentum of re-emitted molecules, corresponding to that of the surface. For most engineering surfaces, it is close to unity. Under controlled test conditions, however, lower accommoda-

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tion coefficients are possible due to the low surface roughness [8]. Sbragaglia and Succi [9] presented a mathematical formulation of kinetic boundary conditions for LB schemes in terms of reflection, slip and accommodation coefficients. In their paper, however, detail investigation and validation using the formula with accommodation coefficient were omitted. Zhang et al. [10] implemented the TMAC to describe the gas-surface interactions in a LB (D2Q9) model. Their boundary condition works in a spirit similar to that of Succi [2]. However, their boundary treatment can only be applied for a stationary wall. Tang et al. [11] presented kinetic theory boundary condition which can be applied for non-fully diffuse wall, and it cannot be adopted only for a stationary wall but also a moving wall. However, it looks somewhat complicated, and it doesn't seem to be easy to use it for a 3D simulation.

The objective of this study is to propose new boundary con ditions for non-fully diffuse wall, and to examine the effect of non-unity accommodation on the slip and the transition flows including the compressible effect of gas flow, which has not been considered in the previous studies mentioned above. For the simulations, 2D/3D gas microchannel flows and oscillatory Couette flow are investigated. dopted only for a stationary wall but also a moving wall.

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the objective of this study is to propose

2. Slip flow regime $(0.01 \leq Kn \leq 0.1)$

2.1 Standard LB method

For a flow without an external force, the following discrete Boltzmann equation is available.

Equations, 2D/3D gas microchannel flows and oscillatory Couette flow are investigated.

\nSlip flow regime (0.01 < Kn < 0.1)

\nStandard LB method

\nFor a flow without an external force, the following discrete
\nlitzmann equation is available.

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\n
$$
\frac{\partial f_a}{\partial t} + e_{ai} \frac{\partial f_a}{\partial x_i} = -\frac{f_a - f_a^{eq}}{\lambda},
$$

\n(1)

\nhere f_a is the particle distribution function, $e_{\alpha i}$ is the micro-

where f_{α} is the particle distribution function, $e_{\alpha i}$ is the microscopic velocity, and λ is the relaxation time. The subscript *i* corresponds to the respective *x*, *y* and *z* directions. The equilibrium distribution function is given by Is, $\angle D/3D$ gas microchannel hows and oscina-
 $\int_a (x + \vec{e}_a \delta t, t + \delta t) - \int_a (x, t)$

regime (0.01 < Kn < 0.1)
 $= \frac{\int_a - \int_a^{\infty} \int_a^{\infty} - \int_a^{\infty} \int_a^{\infty} - \int_a^{\infty} \int_a^{\infty} - \int_a^{\infty} \int_a^{\infty} \int_{(x+\vec{e}_a \delta t, t + \delta t)}^{\infty}$
 \therefore LB *eq i j s ij i j i i ^s ^s e u e e c u u f* $f_a(\vec{x} + \vec{e}_a \delta t, t + \delta t)$
 **Slip flow regime (0.01 < Kn < 0.1)

Standard LB method**

for a flow without an external force, the following discrete the non-dimension is available.

For a flow without an external force, Using
 $-\frac{f_a - f_a^{eq}}{\lambda}$, (1)

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e respective x, y and z di $\frac{\partial f_a}{\partial t} + e_{ai} \frac{\partial f_a}{\partial x_i} = -\frac{f_a - f_a^{eq}}{\lambda}$, (1)
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 \overline{f}_a is the particle distribution function, e_{ai} is the micro-

ic velocity, and λ is the relaxation time. The subscript *i*

esponds to the respec where flow are investigated.
 Solution the investigated.
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 Solution $\int_a (\bar{x} + \bar{e}_a \delta t, t + \delta t) - f_a(\bar{x}, t)$

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and **LB method**

where the non-dimens

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

where t_{α} is a weighting factor, ρ is the density of the system, u_i is the macroscopic velocity, and c_s is the speed of sound. For lattice model, the square lattice (D2Q9) and the 3D 19 velocity (D3Q19) LB models are used for the 2D and 3D sim ulations, respectively [12]. The D2Q9 model has the following set of discrete veloci $z f_a$ is the particle distribution function, e_a is the microcytic and λ is the relaxation time. The subscript i

Eq. (7) can be receast in a s

signosts to the respective x, y and z directions. The equi-
 $\overline{f}_a(\overline{x$

ties:

$$
e_{\alpha} = \begin{cases}\n0 & \alpha = 0 \\
(\cos((\alpha - 1)\pi / 4), \sin((\alpha - 1)\pi / 4)) & \alpha = 1, 3, 5, 7, \\
\sqrt{2}(\cos((\alpha - 1)\pi / 4), \sin((\alpha - 1)\pi / 4)) & \alpha = 2, 4, 6, 8\n\end{cases}
$$
 function is omitted for simplicity.
For rarefied gas simulations, τ in
lated to *Kn*. From the kinetic theory, it
gas molecules, represented by the pa

and the weighting factor t_a is

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$$
d the weighting factor t_a is
$$
\n
$$
t_a = \begin{cases}\n4/9 & \alpha = 0 \\
1/9 & \alpha = 1, 3, 5, 7\n\end{cases}
$$
\n
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t_a = 2, 4, 6, 8
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d = 2, 4, 6, 8
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\n
$$
d = 2, 4, 6, 8
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\n
$$
e_a = \begin{cases}\n0 & \alpha = 0 \\
\alpha = 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1) & \alpha = 1, 2, \dots, 6; \text{ group } I\n\end{cases}
$$

For the D3Q19 model, the discrete velocities e_a and the weighting factor t_a are given by

$$
P(\theta|U) = \frac{1}{2} \int_{\alpha}^{2\pi} \frac{1}{2} \int_{\alpha
$$

$$
\alpha = \begin{cases}\n2/36 & \alpha = 1, 2, ..., 6; \text{ group } I \\
1/36 & \alpha = 7, 8, ..., 18; \text{ group } II\n\end{cases} (6)
$$

time step δt , the following equation can be obtained [9].

(14, 24, 9), (24, 3, 24), (3, 24, 34)
$$
\alpha = 7
$$
, 0,..., 16, *g* only 1
\n $t_{\alpha} =\begin{cases} 12/36 & \alpha = 1, 2, ..., 6; group I . (6) 1/36 & \alpha = 7, 8, ..., 18; group II \end{cases}$
\nThe sound speed c_s is $1/\sqrt{3}$ in both 2D and 3D simulations.
\nBy discretizing Eq. (1) along with the characteristic over the
\nne step $\hat{\alpha}$, the following equation can be obtained [9].
\n $f_{\alpha}(\vec{x} + \vec{e}_{\alpha}\delta t, t + \delta t) - f_{\alpha}(\vec{x}, t)$
\n $= -\frac{f_{\alpha} - f_{\alpha}^{eq}}{2\tau} \Big|_{(\vec{x}, t)} - \frac{f_{\alpha} - f_{\alpha}^{eq}}{2\tau} \Big|_{(\vec{x} + \vec{e}_{\alpha}\delta t, t + \delta t)}$
\nhere the non-dimensional relaxation time $\tau = \lambda/\delta t$.
\nIn the above discretization, the trapezoidal rule is applied to
\ntain the second-order accuracy and unconditional stability.
\nsing the following modified particle distribution function,
\n $\overline{f}_{\alpha} = f_{\alpha} + \frac{f_{\alpha} - f_{\alpha}^{eq}}{2\tau}$. (8)
\nEq. (7) can be recast in a simpler form as follows.
\n $\overline{f}_{\alpha}(\vec{x} + \vec{e}_{\alpha}\delta t, t + \delta t) - \overline{f}_{\alpha}(\vec{x}, t) = -\frac{1}{\tau + 0.5}(\overline{f}_{\alpha} - f_{\alpha}^{eq})|_{(\vec{x}, t)}$ (9)
\nThe macroscopic density, kinematic viscosity, and momen-
\nmer recovered by

where the non-dimensional relaxation time $\tau = \lambda/\delta t$.

In the above discretization, the trapezoidal rule is applied to obtain the second-order accuracy and unconditional stability. Using the following modified particle distribution function, I stability.
 (8)
 (8)
 (9)
 $\frac{1}{(x, t)}$
 d momen-

$$
\overline{f}_\alpha = f_\alpha + \frac{f_\alpha - f_\alpha^{eq}}{2\tau} \,. \tag{8}
$$

$$
\overline{f}_{\alpha}(\vec{x} + \vec{e}_{\alpha}\delta t, t + \delta t) - \overline{f}_{\alpha}(\vec{x}, t) = -\frac{1}{\tau + 0.5}(\overline{f}_{\alpha} - f_{\alpha}^{eq})\Big|_{(\vec{x}, t)}.
$$
 (9)

The macroscopic density, kinematic viscosity, and momentum are recovered by

Now without an external force, the following discrete
\nequation is available.
\nEquation of the equation
$$
\frac{\partial f_a}{\partial x_i} = -\frac{f_a - f_a^{eq}}{\lambda}
$$
,
\n $\frac{\partial f_a}{\partial x_i} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_i} = -\frac{f_a - f_a^{eq}}{\lambda}$,
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\n $\frac{\partial f_a}{\partial x_i} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_i} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_j} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_k} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_k} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_k} = -\frac{f_a - f_a^{eq}}{\lambda}$,
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\n $\frac{\partial f_a}{\partial x_k} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_k} = -\frac{f_a - f_a^{eq}}{\lambda}$,
\n $\frac{\partial f_a}{\partial x_k} = -\frac{f$

Hereafter, the overbar on top of the modified distribution

 $\sqrt{2(\cos((\alpha-1)\pi/4))}$, $\sin((\alpha-1)\pi/4)$ $\alpha = 2, 4, 6, 8$ lated to *Kn*. From the kinetic theory, it can be assumed that the For rarefied gas simulations, τ in Eq. (9) needs to be regas molecules, represented by the particle distribution functions, travel the distance of the lattice mean-free path *l_v* with

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the mean thermal speed defined as $\overline{c} = \sqrt{8kT / \pi m}$ [13] while
 $f_7(x, y, t + \delta t) = \sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$

relaxing to their equ relaxing to their equilibrium state in the relaxation time λ .
The mean thermal speed \overline{c} can be represented with the lattice velocity *c* which depends on the lattice model [12], e.g., *N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4*

the mean thermal speed defined as $\overline{c} = \sqrt{8kT / \pi m}$ [13] while
 $f_7(x, y, t + \delta t) = \sigma f_2(x - \delta t)$

The mean thermal speed \overline{c} can be repre *N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705*

1 thermal speed defined as $\overline{c} = \sqrt{8kT / \pi m}$ [13] while $f_1(x, y, t + \delta t) = \sigma f_2(x - \delta t)$

to their equilibrium state in the relaxation time λ *N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014)*
 c mean thermal speed defined as $\overline{c} = \sqrt{8kT / \pi m}$ [13] while
 c e mean thermal speed \overline{c} can be represented with the lat-
 c velocity *N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4715

thermal speed defined as* $\overline{c} = \sqrt{8kT/\pi m}$ *[13] while* $f_7(x, y, t + \delta t) = \sigma f_2(x - \delta x, y)$ *

to their equilibrium state in the relaxation time N. Jeong / Journal of Mechanical Science and Technology 28 (1) (2014) 4705-4715*

the mean thermal speed defined as $\overline{c} = \sqrt{8kT/\pi m}$ [13] while

The mean thermal speed \overline{c} can be represented with the lat-

tice v

$$
\overline{c} = \sqrt{\frac{8}{3\pi}} c = \sqrt{\frac{8}{3\pi}} \frac{\delta x}{\delta t}.
$$
\n(11)

Therefore, the Knudsen number can be expressed as follows [10]:

$$
Kn = \frac{l_v}{H} = \frac{\lambda \overline{c}}{H} = \sqrt{\frac{8}{3\pi}} \frac{\lambda}{\delta t} \frac{\delta x}{H} = \sqrt{\frac{8}{3\pi}} \frac{\delta x}{H},
$$
 (12) Karlin

inversely dependent on the pressure, the local *Kn* shall be modified as *o* **e** mean thermal speed \overline{c} can be represented with the latt-

velocity *c* which depends on the lattice model [12], e.g.,
 $\overline{c} = \sqrt{\frac{8}{3\pi}} c = \sqrt{\frac{8}{3\pi}} \frac{\delta x}{\delta t}$.

(11) Tang et al. [11]

Tang tal. [11] boun ice velocity c which depends on the lattice model [12], e.g.,
 $\overline{c} = \sqrt{3kT/m}$ for D2Q9 and D3Q19 models.
 $\overline{c} = \sqrt{\frac{8}{3\pi}}c = \sqrt{\frac{8}{3\pi}}\delta x$.
 $\overline{c} = \sqrt{\frac{8}{3\pi}}c\delta x$.
 $\overline{c} = \sqrt{\frac{8}{3\pi}}\delta x$.
 $\overline{c} = \sqrt{\frac{8}{3\pi}}\$

$$
Kn = Kn_o \frac{P_o}{P(x, y)},
$$
\n(13)

tively. The local non-dimensional relaxation time τ is then determined by the local *Kn* .

2.2 Boundary treatments

2.2.1 Previous boundary conditions

The analytic solution in the Boltzmann equation, the distribution function of the gas molecules leaving the wall surface can be related to the incident molecular distribution function by using a scattering kernel. The most widely used kernel is the diffusive scattering model:

$$
\xi(u^{i} \to u) = \frac{m^{2}u_{n}}{2\pi (kT_{w})^{2}} \exp\left(-\frac{mu^{2}}{2kT_{w}}\right),
$$
\n(14) the
\nfirst
\nwhere u^{i} is the incident velocity, u the reflected velocity, T_{w}

the surface temperature, and u_n the normal component of the incident velocity. Maxwell [14] expanded this diffusive kernel to a partially diffusive σ and partially specular (1- σ) kernel. In the LB method, the gas molecule and surface interactions need to be approximated by a combination of the discrete velocities, because the degree of freedom in the momentum space is very limited in the LB method. $\tilde{\xi}(u^i \rightarrow u) = \frac{m^2 u_s}{2\pi (kT_s)^2} \exp\left(-\frac{mu^2}{2kT_s}\right),$ (14) the accommodation coefficient, σ , weighs the friestion and specular reflection. For 2D firstly ereliction and specular reflection. For 2D for the boundary con *f*(*xy* -*xu*) = $\frac{1}{2\pi(kT_y)^2}$ exp₍ - $\frac{1}{2kT_w}$),
 f(*x*) = $\frac{1}{2\pi(kT_y)^2}$ fissive reflection and specular reflection. For 2D
 fore, the boundary condition at the lower wall is a

surface temperature, a

In order to simulate gas microflows, Zhang et al. [10] and Tang et al. [11] used the Maxwellian approach to describe the gas-solid wall collision characteristics. For 2D channel flow, Zhang et al. [10] presented a boundary condition at the upper as follows:

$$
f_{8}(x, y, t + \delta t) = (1 - \sigma) f_{2}(x - \delta x, y, t) , \qquad (12)
$$

$$
f_6(x, y, t + \delta t) = (1 - \sigma) f_4(x + \delta x, y, t) , \qquad (16)
$$

$$
f_7(x, y, t + \delta t) = \sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)
$$

+
$$
f_3(x, y, t)
$$
 (17)

nology 28 (11) (2014) 4705~4715
 $(x, y, t + \delta t) = \sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$
 $+ f_3(x, y, t)$

e σ is the TMAC. This boundary condition doesn't in-

the wall velocity. Their boundary treatment, therefore,

the wall veloc (*14)* 4705-4715
 $f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$, (17)

(*x,y,t*) (17)

(*x, f*₇(*x, y,t* + δt) = $\sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$
 *f*₇(*x, y,t* + δt) = $\sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$

+ $f_3(x, y, t)$

ere σ is the TMAC. This boundary condition doesn't in-

de the wall velocity. T *f x f*₂(*x* - δx , *y*,*t*) + $\sigma f_4(x + \delta x, y, t)$, (17)
*f*₃(*x*, *y*,*t*) (17)
MAC. This boundary condition doesn't in-
locity. Their boundary treatment, therefore, d for a stationary wall.
11 also suggested the 8 (11) (2014) 4705~4715 4707

+ δt) = $\sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$ (17)

+ $f_3(x, y, t)$

the TMAC. This boundary condition doesn't in-

rall velocity. Their boundary treatment, therefore,

analized for a stationary where σ is the TMAC. This boundary condition doesn't include the wall velocity. Their boundary treatment, therefore, can only be applied for a stationary wall.

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mean thermal speed defined as $\overline{c} = \sqrt{8kT/\pi m}$ [13] while
 $f_2(x, y, t + \delta t) = \sigma f_3(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$

where enter the relaxation *H*. *Hennal speed defined as* $\overline{c} = \sqrt{\frac{8}{3\pi}} \frac{\lambda}{c} \frac{\delta x}{\delta t} = \sqrt{\frac{8}{3\pi}} \frac{\delta x}{\delta t}$
 H (content equilibrium state in the relatation time *A*. $f_2(x, y, t + \delta t) = \sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$

to their equilibrium *N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4715

mal speed defined as* $\bar{c} = \sqrt{8kT / \pi m}$ *[13] while
* $f_2(x, y, t + \delta t) = \sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$ *

eir equilibrium state in the relaxat N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4715

dd defined as* $\overline{c} = \sqrt{8kT/\pi m}$ *[13] while
* $f_2(x, y, t + \delta t) = \sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta t)$ *

dibrium state in the relaxation time 2.

depend* which depends on the lattice model [12], e.g.,

or D2Q9 and D3Q19 models.

the context of the TMAC. This

clude the wall velocity. Their

clude the wall velocity. Their

clude the wall velocity. Their

clude the wall velo Tang et al. [11] also suggested the Maxwellian kinetic boundary condition accounting for the TMAC. The unknown distribution function f_α reflected on the wall can be determined by using the incident distribution function f_{α} ^{*'*} and the completely diffusive boundary condition derived by Ansumali and Karlin [15] as follows: for a stationary wall.

also suggested the Maxwellian kinetic

accounting for the TMAC. The unknown
 f_{α} reflected on the wall can be determined

the distribution function $f_{\alpha'}$ and the com-

ndary condition derived nology 28 (11) (2014) 4705-4715

(x, y, t + δt) = $\sigma f_2(x - \delta x, y, t) + \sigma f_4(x + \delta x, y, t)$ (17)
 $+f_3(x, y, t)$ (17)
 $+f_3(x, y, t)$ (17)
 $+f_3(x, y, t)$ (17)

(17)

(are distinguished for a stationary condition doesn't in-

the wall vel 4715 4707
 $(x, y, t) + \sigma f_4(x + \delta x, y, t)$ (17)

is boundary condition doesn't in-

eir boundary treatment, therefore,

it is boundary treatment, therefore,

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umali and
 $(\vec{x}, \rho_w, \vec{u}_w)$

(18)

(18)

(18)

are wall. $(\delta x, y, t) + \sigma f_4(x + \delta x, y, t)$, (17)

is boundary condition doesn't in-

eir boundary treatment, therefore,

tionary wall.

uggested the Maxwellian kinetic

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($\vec{x}, \rho_w, \vec{u}_w$)

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 $+f_3(x, y, t)$ (17)
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 fg $f_3(x, y, t)$ (17)
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 $+f_3(x, y, t)$ (17)

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wall velocity. Their boundary treatment, therefore,
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x, y, t) + $\sigma f_4(x + \delta x, y, t)$, (17)

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Illegested the Maxwellian kinetic

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ted on the wall can be

$$
f_{\alpha}(\vec{x},t+\delta t) = (1-\sigma) f_{\alpha} \cdot (\vec{x},t+\delta t) |(\vec{e}_{\alpha} - \vec{u}_{w}) \cdot \vec{n}| + \sigma \frac{\sum_{(\vec{e}_{\alpha} - \vec{u}_{w}) \cdot \vec{n} \mid (\vec{e}_{\alpha} - \vec{u}_{w}) \cdot \vec{n} |f_{\alpha}(\vec{x},t+\delta t)}{\sum_{(\vec{e}_{\beta} - \vec{u}_{w}) \cdot \vec{n} \mid (\vec{e}_{\beta} - \vec{u}_{w}) \cdot \vec{n} |f_{\beta}^{eq}(\vec{x},\rho_{w},\vec{u}_{w})} f_{\alpha}^{eq}(\vec{x},\rho_{w},\vec{u}_{w})},
$$
(18)

where \vec{u}_w and ρ_w are the velocity and density at the wall.

2.2.2 Present boundary conditions

 $\int_0^L f(x, y) dx$
 $\int f(x) dx$
 $\frac{P_s}{N_x}$, $\frac{P_s}{N_y}$, (13) where \vec{u}_w and ρ_w are the velocity and de P_s are the Kn and pressure at the outlet, respective and ρ_w are the velocity and de P_s are the velocity and and non-dimensional relaxa Kn_o and P_o **i** R_n and P_o are the velocity and defined to $\frac{P_a}{P(x,y)}$, $\frac{P_a}{P(x,y)}$, $\frac{P_a}{P(x,y)}$ **i** $\frac{P_a}{P(x,y)}$ are the velocity and defined by the local Kn **m** is the studied to simulate rarefied gas hows with $I = Kn_o \frac{P_o}{P(x, y)}$, (13) where \vec{u}_w and ρ_w a
 u e Kn_o and P_o are the Kn and pressure at the outlet, respection and \vec{u}_w and \vec{u}_w and \vec{u}_w .

The local non-dimensional relaxation time \vec{r} is the **Fall of the Controllering and the entity of the model of the proposition of the state of the Mandrid (13) where** \vec{u}_w **and** ρ_w **are the velocity and der re the Kn and pressure at the outlet, respectively and the intim** (13)

where \vec{u}_w and ρ_w are the velocity and density

and pressure at the outlet, respec-

2.2.2 Present boundary conditions

usional relaxation time τ is then

In this study, two different boundary condi

geste $Kn_o \frac{P_o}{P(x, y)},$
 $Kn_o \frac{P_o}{P(x, y)},$
 $\frac{P_o}{P(x, y)}$, and P_o are the velocity and density
 $\frac{P_o}{P(x, y)}$, and P_o are the velocity and density

The local non-dimensional relaxation time *r* is then

In this study, two dif (13)

where \vec{u}_w and ρ_w are the velocity and density

and pressure at the outlet, respec-

2.2.2 Present boundary conditions

sional relaxation time τ is then

In this study, two different boundary condi

gested In this study, two different boundary conditions are suggested to simulate rarefied gas flows with non-fully diffuse walls. The first one is a combination of the wall equilibrium and the free-slip boundary conditions. Using the equilibrium distribution function as a boundary condition of the LBE method is to assume that the reflection of molecules impinging on the wall is fully diffuse (σ = 1). On the other hand, free-slip boundary condition [16] applies to the case of smooth boundaries without friction, and it represents a specular reflection (σ = 0), i.e. the incoming particles to the wall are reflected as light is reflected from a mirror after the collision. The nonfully diffuse reflection may lie between these two limits, and the accommodation coefficient, σ , weighs the fraction of diffusive reflection and specular reflection. For 2D case, therefore, the boundary condition at the lower wall is as follows for a non-fully diffuse wall: n this study, two different boundary conditions are sug-
ted to simulate rarefied gas flows with non-fully diffuse
ls. The first one is a combination of the wall equilibrium
the free-slip boundary conditions. Using the eq Is. The first one is a combination of the wall equilibrium
the free-slip boundary conditions. Using the equilibrium
infusion function as a boundary condition of the LBE
hold is to assume that the reflection of molecules the free-slip boundary conditions. Using the equilibrium
ribution function as a boundary condition of the LBE
hold is to assume that the reflection of molecules imping-
on the wall is fully diffuse ($\sigma = 1$). On the other

$$
f_2(x, y, t + \delta t) = \sigma f_2^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_8(x - \delta x, y + \delta x, t),
$$
\n(19)
\n
$$
f_3(x, y, t + \delta t) = \sigma f_3^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_7(x, y + \delta x, t),
$$
\n(20)
\n
$$
f_4(x, y, t + \delta t) = \sigma f_4^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_6(x + \delta x, y + \delta x, t).
$$
\n(21)

For a stationary wall, $\vec{u}_w = 0$, and the density is obtained by taking the zeroth moment of the particle distribution function at the wall after the streaming step. Wall boundaries are located halfway between two grid points.

The other boundary condition can be derived by using specular bounce-back scheme for diffusive reflection, which can be presented as follows:

$$
f_2(x, y, t) = rf_6(x, y, t) + (1 - r)f_8(x, y, t) ,
$$
\n(22)

$$
f_3(x, y, t) = f_7(x, y, t), \qquad (23)
$$

$$
f_4(x, y, t) = rf_8(x, y, t) + (1 - r)f_6(x, y, t) ,
$$
\n(24)

N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4715
 *f*₂(*x, y,t*) = $rf_6(x, y, t) + (1 - r)f_8(x, y, t)$, (22) pressure:
 *f*₃(*x,y,t*) = $f_7(x, y, t)$, (23) $1 - \tilde{P}^2 + 12 \times 1.11 \frac{2 - \sigma}{\sigma} K n_o (1 -$ *N. Jeong* / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4715
 *f*₂(*x, y,t*) = $rf_6(x, y, t) + (1 - r)f_8(x, y, t)$, (22) pressure:
 $f_3(x, y, t) = f_7(x, y, t)$, (23) $1 - \tilde{P}^2 + 12 \times 1.11 \frac{2 - \sigma}{\sigma} K n_0 (1 - \tilde{P})$ where r is the specular factor. The sum of x-momentum for reemitted particles from the bottom wall after the collision is as where *r* is the specular factor. The sum of x-momentum for re-
emitted particles from the bottom wall after the collision is as
follows:
 $J_x = f_2 - f_4 = (1 - 2r)(f_8 - f_6) = \frac{\rho}{6}u_w$, (25)
and
and
 $r = \frac{1}{2} - \frac{\rho}{12} \frac{u_w}{f_8 - f$

$$
J_x = f_2 - f_4 = (1 - 2r)(f_8 - f_6) = \frac{\rho}{6}u_w,
$$
\n(25)

$$
r = \frac{1}{2} - \frac{\rho}{12} \frac{u_w}{f_8 - f_6} \,. \tag{26}
$$

N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014
 x, y, t) = $f_6(x, y, t) + (1 - r) f_8(x, y, t)$,
 z, y, t) = $f_5(x, y, t)$,
 z, y, t) = $f_5(x, y, t) + (1 - r) f_6(x, y, t)$,
 z (23) $1 - \tilde{P}^2 + 12 \times 1.11 \frac{2 - \tilde{P}}{\$ *M. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4*
 *f*₈(*x, y,t*) + (1-*r*) $f_s(x, y, t)$, (22) pressure:

(23) $1 - \bar{P}^2 + 12 \times 1.11 \frac{2 - \sigma}{\sigma} K n_o(1 - \sigma) K (x, y, t)$ (24)

specular factor. The su *N. Jeong* / Journal of Mechanical Science and Technology 28 (11) (20

(x, y,t) = $rf_6(x, y, t) + (1 - r)f_8(x, y, t)$,

(22) pressure:

(x, y,t) = $f_5(x, y, t) + (1 - r)f_6(x, y, t)$,

(23) $1 - \bar{P}^2 + 12 \times 1.11 \frac{2}{r}$

(x, y,t) = $rf_9(x, y, t$ If a stationary wall is considered, r should be 0.5, and J_x becomes 0, which means diffuse reflection, i.e. the particles reflected back diffusively from the wall without a certain an gle of reflection. Thus, non-fully diffuse reflection can be possibly achieved by following boundary condition:

$$
f_2(x, y, t) = r \sigma f_6(x, y, t) + (1 - r \sigma) f_8(x, y, t) , \qquad (27)
$$

$$
f_3(x, y, t) = f_7(x, y, t), \tag{28}
$$

$$
f_4(x, y, t) = r \sigma f_8(x, y, t) + (1 - r \sigma) f_6(x, y, t) . \tag{29}
$$

Wall boundaries are also located halfway between two grid points.

2.3 Numerical simulation

2.3.1 2D microchannel flow

The analytic solution of a microchannel flow between two parallel plates of length *L*, which are separated apart by a distance *H*, can be deduced from the Navier-Stokes equation using the slip boundary condition. When the second-order slip model is considered, the slip velocity is

$$
u_s - u_{\text{wall}} = \alpha \frac{2 - \sigma}{\sigma} l \frac{\partial u}{\partial n}\bigg|_{\text{wall}} - \beta l^2 \frac{\partial^2 u}{\partial n^2}\bigg|_{\text{wall}},
$$
(30)

where u_s and n are the slip velocity and wall normal coordinate, and *uwall* denotes the wall velocity. For a flat wall, Hadjiconstantinou [17] has been proposed the slip coefficients α = 1.11 and β = 0.61 from the accurate numerical solutions of the Boltzmann equation. Under the assumption of a long channel, i.e. $L/H \gg 1$, the following analytical solutions can be deduced with Eq. (30) [18]. llel plates of length L, which are separated apart by a dis-

The results of previous boundary treatments show lower value
 H , can be educed from the Navier-Sluskes equation uses of the stip velocity and nonlinearity of *H* analyso solution to a intervel intervel of the same *H* and $V = 0.4$ and $V = 0.5$ and $V = 0.7$ and $V = 0.4$ and *d* is some *diagral*, when the signarion was self-
to deduced from the Navier-Stokes equation
be deduced from the Navier-Stokes equation
oundary condition. When the second-order slip compared with the analytical solution Leaded from the Navicus and the space of the space of α , α and α are α of α is α and α are estimated above that Navicus Sc Eventual of the Navier-Stokes equation

deduced from the Navier-Stokes equation

deduced from the Navier-Stokes equation

or of the slip velocity and nonlinearity

dary condition. When the second-order slip

compared with

velocity:
\n
$$
u(y) = -\frac{H^2}{2\mu} \frac{dP}{dx} \left[-\left(\frac{y^2}{H^2}\right) + \left(\frac{y}{H}\right) + 1.11 \frac{2 - \sigma}{\sigma} K n + 2 \times 0.61 K n^2 \right],
$$
\nwhere\n
$$
F_a = \left(1 - \frac{1}{2\tau + 1}\right) t_a
$$
\n
$$
(31)
$$

pressure:

8
\n8
\n
$$
N. \text{Jeong } / \text{Journal of Mechanical Science and Technology } 28 (11) (2014) 4705-4715
$$
\n
$$
f_2(x, y, t) = rf_6(x, y, t) + (1 - r) f_8(x, y, t),
$$
\n
$$
f_3(x, y, t) = f_7(x, y, t),
$$
\n
$$
f_4(x, y, t) = rf_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_5(x, y, t) = rf_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_6(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_7(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_8(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
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\n
$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
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f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
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$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
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\n
$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_9(x, y, t) = T_8(x, y, t) + (1 - r) f_6(x, y, t),
$$
\n
$$
f_9(x, y, t) =
$$

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pressure:
* $1 - \tilde{P}^2 + 12 \times 1.11 \frac{2 - \sigma}{\sigma} K n_o (1 - \tilde{P}) - 24 \times 0.61 K n_o^2 \ln \tilde{P} = B(1 - \tilde{x})$ *,

(32)

where <i>R* is the gas constant; $\tilde{P} = P/P_o$, the normalized pressure with the o where R is the gas constant; $\tilde{P} = P/P_a$, the normalized pressure with the outlet pressure; *x x L* % ⁼ / , the coordinate nor- malized with the channel length; and *B* a constant such that $\tilde{P}(0) = P/P$.

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 N. Jeong / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4715
 $f_2(x, y, t) = f'_6(x, y, t) + (1 - r) f_s(x, y, t)$,

(22) pressure:
 $f_3(x, y, t) = f_5(x, y, t) + (1 - r) f_6(x, y, t)$,

(23) $1 - \tilde{P}^2 + 12 \times 1.11 \frac{2 - \sigma}{\sigma}$ *x x*, *y*, *i* = $f'_k(x, y, t) = f'_k(x, y, t) + (1 - r) f'_s(x, y, t)$,
 $f'_2(x, y, t) = f'_f(x, y, t) + (1 - r) f'_s(x, y, t)$,
 $f'_k(x, y, t) = f'_k(x, y, t) + (1 - r) f'_s(x, y, t)$,

(22)

pressure:
 $f'_k(x, y, t) = f'_k(x, y, t) + (1 - r) f_s(x, y, t)$,

(22)
 $1 - \bar{P}^2 + 12 \times 1.11 \frac$ *N. Jeong* / Journal of Mechanical Science and Technology 28 (11) (2014) 4705-4715
 x, y,t) = $f_6(x, y, t) + (1 - r) f_8(x, y, t)$,

(22) pressure:
 x,y,t) = $f_5(x, y, t) + (1 - r) f_6(x, y, t)$,

(23) $1 - \tilde{P}^2 + 12 \times 1.11 \frac{2 - \sigma}{\sigma} K n$ Technology 28 (11) (2014) 4705-4715

pressure:
 $1 - \bar{P}^2 + 12 \times 1.11 \frac{2-\sigma}{\sigma} K n_o (1-\bar{P}) - 24 \times 0.61 K n_o^2 \ln \bar{P} = B(1-\bar{x})$,

(32)

where *R* is the gas constant; $\bar{P} = P/P_o$, the normalized pres-

sure with the outlet pres The unknown particle distribution functions at the inlet and outlet are calculated by second-order extrapolation of those adjacent to the boundary nodes. Following the extrapolation, the calculated densities at the inlet and outlet are rescaled to make the average density across the inlet and outlet boundary nodes the same as the prescribed density.

f x y t r f x y t r f x y t (, ,) (, ,) (1) (, ,) ⁼ ^s + - ^s , (27) ³ ⁷ ows:

sure with the outlet pressure; \dot{x} maized with the outlet pressure; \dot{x} maized with the channel length;
 $f_x = f_2 - f_4 = (1 - 2r)(f_8 - f_6) = \frac{\rho}{6}u_v$,
 $\dot{f}(0) = P_i / P_o$. The unknown particle distribution the boundary *f x y t r f x y t r f x y t* (, ,) (, ,) (1) (, ,) ⁼ ^s + - ^s . (29) *s*(*x, y,t*) = $r\sigma f_s(x, y, t) + (1 - r\sigma) f_s(x, y, t)$, and the pressure rom the 1)
 P_{anom} and the pressure rom the 1)
 $\int_{s}^{x} f_s(x, y, t) = f_s(x, y, t) + (1 - r\sigma) f_s(x, y, t)$. (27) distribution, $(P - P_{anom}$), is normalized by the
 $\int_{s}^{x} f$ *f₃*(*x, y,t*) = $r\sigma f_n(x, y, t) + (1 - r\sigma) f_n(x, y, t)$ (27) distribution, $(P - P_{known})$, is normalized by the $f_3(x, y, t) = f_3(x, y, t)$, (28) P_n and the stream direction, in an *x* condinate:
 u $f_4(x, y, t) = r\sigma f_n(x, y, t) + (1 - r\sigma) f_n(x, y, t$ $(x, y, t) = r\sigma f_6(x, y, t) + (1 - r\sigma) f_8(x, y, t)$,
 $\sigma f_9(x, y, t) = (1 - r\sigma) f_8(x, y, t)$,
 $\sigma f_9(x, y, t) = r\sigma f_8(x, y, t) + (1 - r\sigma) f_9(x, y, t)$.
 $\sigma f_9(x, y, t) = r\sigma f_8(x, y, t) + (1 - r\sigma) f_9(x, y, t)$.
 $\sigma f_9(x, y, t) = r\sigma f_8(x, y, t) + (1 - r\sigma) f_9(x, y, t)$.
 $\sigma f_9(x, y$ y,t)+(1-r σ) $f_s(x, y, t)$, (27)

(27) Ensumbuton, ($t^2 - r_{infty}$), sommalized by the parameterion, in an x coordinal
 σ ,t)+(1-r σ) $f_s(x, y, t)$. (28) σ , and the stream direction, in an x coordinal

by the channel length Fig. 1 shows the results for $Kn_0 = 0.05, 0.1$ and $\sigma = 0.9, 0.6$ compared with the analytical solutions of Eqs. (31) and (32). The grid size for *H* is restricted to 30 δx (32 points), and L/H = 80 is used in order to investigate the compressibility and rarefaction effects on a sufficiently long micro-channel flow. For all calculations, P_i/P_o is set to 2.0. The nonlinearity of pressure, i.e. deviation of the pressure from the linear pressure distribution, $(P - P_{incomp.})$, is normalized by the outlet pressure, *P^o* , and the stream direction, in an *x* coordinate, is normalized by the channel length. Slip velocities are normalized by the outlet centerline velocity *U^o* . The results are same for both boundary treatments, and they are also in excellent agreement with the analytical solutions. That shows that non-fully diffuse reflection can be successfully achieved by linear combination of fully diffuse and specular reflections, and the wall equilibrium boundary condition and the specular bounce-back scheme with $r = 0.5$ represent the diffuse reflection well.

For the comparison with the previous boundary treatments, the results for $Kn_o = 0.1$ and $\sigma = 0.9$ are presented in Fig. 2. The results of previous boundary treatments show lower values of the slip velocity and nonlinearity of pressure when compared with the analytical solutions.

To evaluate the effect of grid size on the accuracy of the solutions, the gas flows in an infinitely long microchannel are studied.

In order to mimic the flow, a periodic microchannel flow driven by a constant external pressure gradient is considered. In the presence of a body force, the LB must be modified to account for the force by adding an additional term to Eq. (9). boundary teaments, and they are also in exceleint agreement
with the analytical solutions. That shows that non-fully diffuse
reflection can be successfully achieved by linear combination
of fully diffuse and specular refl $\vec{F} = \rho \vec{g}$, where \vec{g} is the acceleration, is as follows [19]: channel are

annel flow

considered.

modified to

to Eq. (9).
 $\rho \vec{g}$, where
 $+ \delta t F_{\alpha}$,

(33) If we are a spectra rections, and the special renew with $r = 0.5$ represent the diffuse reflection well.

the comparison with the previous boundary treatments,

ne with $r = 0.5$ represent the diffuse reflection well.

the *x* the boundary dimension and the specular boundary condition and the specular boundary condition and the specular boundary treatments, results for $Kn_a = 0.1$ and $\sigma = 0.9$ are presented in Fig. 2. results of *r*ewisos bo the and spectrum and the spectral boundaries, and the wave and equino-
that are variable and the specular bounce-back
 $h = 0.5$ represent the diffuse reflection well.
omparison with the previous boundary treatments,
for Kn unuse and spectrual releations, and we wan equino-
oundary condition and the specular bounce-back
with $r = 0.5$ represent the diffuse reflection well.
le comparison with the previous boundary treatments,
lts for $Kn_o = 0.1$ for the successium and speed of mean combination
of three and speeduar reflections, and the wall equilib-
boundary condition and the specular bounce-back
e with $r = 0.5$ represent the diffuse reflection well.
the comparis the slip velocity and nonlinearity of pressure when

d with the analytical solutions.

luate the effect of grid size on the accuracy of the so-

he gas flows in an infinitely long microchannel flow

y a constant external is of the slip velocity and nonlinearity of pressure when
mpared with the analytical solutions.

for evaluate the effect of grid size on the accuracy of the so-

for evaluate the effect of grid size on the accuracy of the ical solutions.

of grid size on the accuracy of the so-

an infinitely long microchannel are

thow, a periodic microchannel flow

ernal pressure gradient is considered.

by force, the LB must be modified to

adding an ad f the slip velocity and nonlinearity of pressure when
red with the analytical solutions.
waluate the effect of grid size on the accuracy of the so-
s, the gas flows in an infinitely long microchannel are
d.
d.
toret to mi this of previous boundary treatments show lower val-
the slip velocity and nonlinearity of pressure when
d with the analytical solutions.
the slap velocity and nonlinearity of pressure when
datate the effect of grid size

$$
\overline{f}_a(\vec{x} + \vec{e}_a \delta t, t + \delta t) - \overline{f}_a(\vec{x}, t) = -\frac{1}{\tau + 0.5} (\overline{f}_a - f_a^{eq}) \Big|_{(\vec{x}, t)} + \delta t F_a,
$$
\n(33)

where

$$
F_{\alpha} = \left(1 - \frac{1}{2\tau + 1}\right) t_{\alpha} \left[\frac{\vec{e}_{\alpha} - \vec{u}}{c_s^2} + \frac{(\vec{e}_{\alpha} \cdot \vec{u})}{c_s^4} \vec{e}_{\alpha}\right] \cdot \vec{F} \tag{34}
$$

(a) Nonlinearity of pressure normalized by the outlet pressure

(b) Slip velocity normalized by the outlet centerline velocity

Fig. 1. Nonlinearity of pressure and slip velocity distributions for $Kn_0 = 0.05$, 0.1 and $\sigma = 0.9$, 0.6 at $P_f/P_o = 2.0$, $H = 30 \frac{\partial x}{\partial x}$, and $L/H = 80$.

 (a) Nonlinearity of pressure normalized by the outlet pressure (b) Slip velocity normalized by the outlet centerline velocity Fig. 2. Nonlinearity of pressure and slip velocity distributions of previous boundary treatments for $Kn_o = 0.1$ and $\sigma = 0.9$.

(a) Combination of wall equilibrium and free-slip condition

(b) Combination of specular bounce-back and free-slip condition.

Fig. 3 shows the velocity profiles for the cases of $H = 10\delta x$, $20\delta x$, $40\delta x$, and $80\delta x$ when $Kn = 0.1$ and $\sigma = 0.8$. The results are non-dimensionalized by the mean velocity *Um*,

$$
U_m = -\frac{H^2}{2\mu} \frac{dP}{dx} \left[\frac{1}{6} + 1.11 \frac{2 - \sigma}{\sigma} K n + 2 \times 0.61 K n^2 \right].
$$
 (35) and $\xi = \sqrt{i} S$.

It is seen that the accuracy of the solutions is essentially in dependent of the grid size for both boundary conditions.

2.3.2 Oscillatory shear-driven gas flow

The schematic diagram of the oscillatory Couette flow is presented in Fig. 4. The lower plate at $y = 0$ is a stationary wall and the upper plate at $y = H$ is a moving wall. At time $t =$ 0, the upper plate starts to oscillate in the *x* direction with velocity $u = u_w \sin(\omega t)$. ω is the oscillation frequency and u_w is the velocity amplitude.

Oscillatory Couette flow is characterized by the Stokes

Fig. 4. Schematic diagram of the oscillatory Couette flow.

number *S*, which represents balance between the unsteady and *v*
 y=*H*
 y=*O*
 y=*O*
 y
 y=*O*
 y=*C*
 y=*C*
 y=*C*
 y=*C*
 y=*C*
 y= rarefied flow are as follows: **y/H** $y=H$
 $\xrightarrow{u=u_v\sin(vt)}$
 $y=0$
 $y=0$
 $\xrightarrow{y=0}$
 $\xrightarrow{y=0}$
 $\xrightarrow{2x}$

2.4. Schematic diagram of the oscillatory Couette flow.

mber *S*, which represents balance between the unsteady and

cous effects, defined as $S = \sqrt{\$ *y*=*H*
 y=*H*
 y solution of the oscillatory Couette flow.
 y solution of the oscillatory Couette flow.
 y solution for the Couette flow problem is

selfiects, defined as $S = \sqrt{\omega H^2 / \nu}$. The reduced Na-

okes *y* $y=0$
 $y=0$
 w $y=0$
 w w u u n u n e s **s** *s v w d i v n u n e n u n counts e f n a -s ioon ior for e Couette flow problem* is $\frac{1}{2}a + v^2u / v^2$, an *y* sagram of the oscillatory Couette flow.

represents balance between the unsteady and

leftined as $S = \sqrt{\omega H^2 / v}$. The reduced Nation for the Couette flow problem is

², and boundary conditions for oscillatory

², $y=0$
 $y=0$
 $\Rightarrow x$

Ber S, which represents balance between the unsteady and

bus effects, defined as $S = \sqrt{\omega H^2 / \nu}$. The reduced Na-

Stokes equation for the Couette flow problem is
 $\partial t = v\partial^2 u / \partial y^2$, and boundary co atory Couette flow.

the between the unsteady and
 $\omega H^2 / \nu$. The reduced Na-

Couette flow problem is

y conditions for oscillatory

(36)
 $\frac{\partial u}{\partial y} + \beta l^2 \frac{\partial^2 u}{\partial y^2}$. (37)

0]

8 sinh $\left(\xi \frac{H - y}{H}\right)$ exp(iot) $\$ mber *S*, which represents balance between the unsteady and

cous effects, defined as $S = \sqrt{\omega H^2 / v}$. The reduced Na-
 T-Stokes equation for the Couette flow problem is
 $\frac{\partial f}{\partial t} = v\partial^2 u / \partial y^2$, and boundary condition *S*, which represents balance between the unsteady and
effects, defined as $S = \sqrt{\omega H^2 / \nu}$. The reduced Na-
kes equation for the Couette flow problem is
 $= v\partial^2 u / \partial y^2$, and boundary conditions for oscillatory
flow are as hich represents balance between the unsteady and

ets, defined as $S = \sqrt{\omega H^2 / v}$. The reduced Na-

equation for the Couette flow problem is
 $u / \partial y^2$, and boundary conditions for oscillatory

are as follows:
 $\sigma_l \frac{\partial u}{\$ $\frac{1}{0.5}$ $\frac{1}{20}$ $\frac{1}{0.5}$ $\frac{1}{20}$ $\frac{1}{0.5}$ $\frac{1}{0$ **Equilibrium+Free-slip(H=80** δ x)
viscous effects, defined as $S = \sqrt{\omega H^2 / v}$. The reduced Na-

at
$$
y = 0
$$
:
\n
$$
u = \alpha \frac{2 - \sigma}{\sigma} l \frac{\partial u}{\partial y} - \beta l^2 \frac{\partial^2 u}{\partial y^2}
$$
\n(36)

at
$$
y = H
$$
:
\n
$$
u - u_w \operatorname{Im}[\exp(i\omega t)] = -\alpha \frac{2 - \sigma}{\sigma} l \frac{\partial u}{\partial y} + \beta l^2 \frac{\partial^2 u}{\partial y^2}.
$$
\n(37)

at
$$
y = 0
$$
:
\n $u = \alpha \frac{2-\sigma}{\sigma} l \frac{\partial u}{\partial y} - \beta l^2 \frac{\partial^2 u}{\partial y^2}$ (36)
\nat $y = H$:
\n $u - u_w \text{Im}[\exp(i\omega t)] = -\alpha \frac{2-\sigma}{\sigma} l \frac{\partial u}{\partial y} + \beta l^2 \frac{\partial^2 u}{\partial y^2}$ (37)
\nThe solution is then given by [20]
\n $u(y) = \text{Im} \left\{ \left[A \cosh \left(\xi \frac{H-y}{H} \right) + B \sinh \left(\xi \frac{H-y}{H} \right) \right] \exp(i\omega t) \right\},$ (38)
\nhere
\n
$$
A = u_w \frac{C_2}{\left(1 + \beta \xi^2 K n^2 \right) C_2 + \alpha \frac{2-\sigma}{\sigma} \xi K n C_1}
$$
 (39)
\n
$$
B = -\frac{C_1}{C_2} A
$$
 (40)
\n $C_1 = \cosh \xi + \alpha \frac{2-\sigma}{\sigma} \xi K n \cdot \sinh \xi + \beta \xi^2 K n^2 \cosh \xi$ (41)
\n $C_2 = \sinh \xi + \alpha \frac{2-\sigma}{\sigma} \xi K n \cdot \cosh \xi + \beta \xi^2 K n^2 \sinh \xi$ (42)
\nd $\xi = \sqrt{i}S$.
\nThe periodic boundary condition is applied in the *x* direc-
\nn. The oscillation frequency can be related with non-
\nnensional period T_p as $\omega = 2\pi/(T_p \delta)$. In Fig. 5, the com-

where

$$
A = u_w \frac{C_2}{\left(1 + \beta \xi^2 K n^2\right) C_2 + \alpha \frac{2 - \sigma}{\sigma} \xi K n C_1}
$$
(39)

$$
B = -\frac{C_1}{C_2}A\tag{40}
$$

$$
C_1 = \cosh \xi + \alpha \frac{2 - \sigma}{\sigma} \xi K n \cdot \sinh \xi + \beta \xi^2 K n^2 \cosh \xi \tag{41}
$$

$$
C_2 = \sinh \xi + \alpha \frac{2 - \sigma}{\sigma} \xi K n \cdot \cosh \xi + \beta \xi^2 K n^2 \sinh \xi \tag{42}
$$

The periodic boundary condition is applied in the *x* direction. The oscillation frequency can be related with non dimensional period T_p as $\omega = 2\pi/(T_p\delta t)$. In Fig. 5, the comparison of the dynamic velocity profiles for $\sigma = 0.9$; $\sigma = 0.5$, and $Kn = 0.05$; $Kn = 0.1$ is shown. For all calculations, *S* is fixed to 4.0. It is seen that the present results are in excellent agreement with those of analytical solutions. In addition, the symbols which represent the results of two boundary treatments are located on the same positions.

2.3.3 3D microchannel flow

In order to examine that the present boundary treatments are

Fig. 5. Non-dimensional dynamic velocity profiles for $\sigma = 0.9$; $\sigma = 0.5$, and $Kn = 0.05$; $Kn = 0.1$.

Fig. 6. Non-dimensional velocity profile of 3D microchannel flow for *Kn* = 0.1 and *Ar* = 0.5.

also applicable in a 3D simulation, 3D gas microchannel flow and it is assumed that $H \leq W$. Under the assumption of a long channel, i.e. $W, H \ll L$, and a locally fully developed flow, i.e. the density ρ and the pressure *P* are constant within a cross section, the steady compressible gas flow in a cross section is governed by the conservation and momentum equations: mulated. The length of the channel is L, its width is $2W$,
its depth is 2H, so that $z \in \{0, L\}$, $x \in \{-W, W\}$, and
 $\{-H, H\}$. The aspect ratio of the cross section is $Ar = H/W$,
it is assumed that $H \le W$. Under the assumpt is depth is 2*H*, so that $z \in \{0, L\}$, $x \in \{-W, W\}$
 $-H, H\}$. The aspect ratio of the cross section is $Ar =$

is assumed that $H \le W$. Under the assumption of z

iel, i.e. $W, H \le L$, and a locally fully developed flow

en . Non-dimensional velocity profile of 3D microchannel flow for $Kn = 0.1$ and $Ar = 0.5$.
 und $\alpha = 0.9$ (b) $\sigma = 0.9$
 $\alpha = 0.9$

(c) $\sigma = 0.9$
 undated. The length of the channel is *L*, its width is 2*W*,
 $\alpha = -H, H$). *y x dz* ^m 6
 Example 18

(a) $\sigma = 0.9$

(b) it is septh is 2H, s ⁰ ^{0.25} **xW** or y_W ^{0.75} ¹ ⁰ ^{0.25} (a) $\sigma = 0.9$ (b)

Non-dimensional velocity profile of 3D microchannel flow for $Kn = 0.1$ and $Ar = 0.5$.

plicable in a 3D simulation, 3D gas microchannel flow Fig. 6 shows the **EXECUTE:** (a) $\sigma = 0.9$

(a) simulation, 3D gas microchannel flow for $Kn = 0.1$ and $Ar = 0.5$.

Complicable in a 3D simulation, 3D gas microchannel for Fig. 6 sho

$$
\frac{\partial u}{\partial z} = 0\tag{43}
$$

$$
\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial x^2} = \frac{1}{\mu} \frac{dP}{dz}.
$$
 (44)

For the simulation of infinitely long channel, Eq. (33) and periodic boundary condition in *z* direction are applied.

Fig. 6 shows the velocity profiles non-dimensionalized by the mean velocity, $U_m = \frac{1}{A} \int_A u(x, y) dA$, for $Kn = 0.1$ and Ar $= 0.5$. Two cases of $\sigma = 0.9$ and 0.6 are considered to see the non-unity accommodation effect. The results are compared with those of the analytical solution derived by Aubert and Colin [21]. They presented the solution based on a double Fourier series using the second-order slip model proposed by Deissler [22]. The results of present study are in very good agreement with the analytical solutions even for the case of quite smooth wall. The deviation between the results of two boundary conditions is negligible.

The simulations for a long 3D microchannel, which has finite length, are also carried out. $400\alpha x$, $20\alpha x$, and $10\alpha x$ are used for *L*, *W* and *H*, respectively. Figs. 7(a) and (b) show the velocity contours at the side wall and bottom wall when *Kn^o* = 0.1, and $\sigma = 0.9$; $\sigma = 0.6$, respectively. The slip velocity at the

Fig. 7. Velocity contours at the side wall and bottom wall of a long 3D microchannel.

side wall becomes larger than that of bottom wall. The differ ence comes from variation in the shear rate along the walls. Consequently, the slip velocity distribution in 3D gas microchannel flow is much more complicated than its 2D counter part, which assumes the velocity profile to be a simple combination of a parabolic velocity profile and a known slip velocity.

3. Transition flow regime $(0.1 \leq Kn \leq 1)$

3.1 High order LB method

When the Knudsen number becomes larger than 0.1, the real velocity profile distinctly deviates from the one predicted by the standard LB model because of the Knudsen layer effect near the wall. To capture the flow characteristics in the Knudsen layer, high order LB model should be adopted. Tang et al. [23] showed following D2Q13 model can predict flow in the transition regime. comes larger than that of bottom wall. The differ-
 $(L_2y)l_A$ or moving towards $y = L$. The local mean free pain of

from variation in the shear rate along the walls.

if modecules can be determined by averaging these two **example the particle distribution and the observed by the different** $(L_2)f/d$ **, for** *n* **owards give L. The local mean free particle and the particle and the set are nones from a transition in the shear rate along the walls B method** the free-slip particle dist

particle dist

dsen number becomes larger than 0.1, the re-

distinctly deviates from the one predicted by condition at

model because of the Knudsen layer effect

capture the flow **High order LB method**

7hen the Knudsen number becomes larger than 0.1

2locity profile distinctly deviates from the one pred

standard LB model because of the Knudsen layer

1. To capture the flow characteristics in the omes from variation in the shear rate along the walls. all molecules can be determined by averaging these two
upution in the shear rate along the walls. all molecules can be determined by averaging these two
upution if a part, which assumes the velocity profile to be a simple combi-
aation of a parabolic velocity profile and a known slip velocity.
3. **Transition flow regime (0.1 < Kn < 1)** For the case of the combination of the the studie particle distribution function f_{0} needs to be added

the Knudsen number becomes larger than 0.1, the re-

cos(file distinctly deviates from the one predicted by

condition at the lower vall is as follows:

and LB mode is Knutsen intendent Peconomis larger than 0.1, the re-

profile distinctly deviates from the one predicted by

profile distinctly deviates from the one predicted by

condition at the lower wall is as follows:

and LB mod promotes since the predicted by
 πP (1), sin((α -1) π /4)) ar = 0, 10,11,12

(oos((α -1) π /4), sin((α -1) π /4)) ar = 9,10,11,12
 \int_{2}^{2} (x, sin((α -1) π /4)) ar = 9,10,11,12
 \int_{2}^{2} (x, sin((α -1) particle distribution function f_0 needs to be add

udsen number becomes larger than 0.1, the re-

lele distinctly deviates from the one predicted by

condition at the lower vall is as follows:

B model because of the K dsen number becomes larger than 0.1, the re-

distinctly deviates from the one predicted by

and distinctly deviates from the one predicted by

model because of the Knudsen layer effect

capture the flow characteristics i e distinctly averages romation at the lower wall is as follows:

andel because of the Knudsen layer effect

capture the flow characteristics in the Knud

order LB model should be adopted. Tang et al.

lowing D2Q13 model c

$$
f_{\alpha}^{eq} = t_{\alpha} \rho \left[1 + \frac{e_{\alpha i} u_i}{c_s^2} + \frac{(e_{\alpha i} u_i)^2}{2c_s^4} - \frac{u_i u_i}{2c_s^2} + \frac{(e_{\alpha i} u_i)^3}{2c_s^6} - \frac{3(e_{\alpha i} u_i)(u_i u_i)}{2c_s^4} \right] \qquad f_4(x, y, t + \delta t) = \sigma f_4(x, y, t + \delta t)
$$

(45) $f_{10}(x, y, t + \delta t) = \sigma f_4(x, y, t + \delta t)$

ties:

$$
e_{\alpha} = \begin{cases}\n0 & \alpha = 0 \\
\cos((\alpha - 1)\pi / 4), \sin((\alpha - 1)\pi / 4)) & \alpha = 1, 3, 5, 7 \\
\sqrt{2}(\cos((\alpha - 1)\pi / 4), \sin((\alpha - 1)\pi / 4)) & \alpha = 2, 4, 6, 8 \\
2(\cos((\alpha - 1)\pi / 4), \sin((\alpha - 1)\pi / 4)) & \alpha = 9, 10, 11, 12 \\
d_{\alpha} = 9, 10, 11, 12 & J_x = f_2 - f_4 = (1 - 2r)(f_8 - f_6) = (46)\n\end{cases}
$$

and the weighting factor t_a is

channel Science and Technology 28 (11) (2014) 4705–4715

\nand the weighting factor
$$
t_{\alpha}
$$
 is

\nand the weighting factor t_{α} is

\n
$$
t_{\alpha} = \begin{cases} 3/8 & \alpha = 0 \\ 1/16 & \alpha = 2, 4, 6, 8 \\ 1/96 & \alpha = 9, 10, 11, 12 \end{cases}
$$
\nTo consider the Knudsen layer effect, the local relaxation time should be determined, and can be related with the local mean free path as follows [24]:

\n
$$
\tau = \frac{l}{l_o} \sqrt{\frac{\pi}{8}} \frac{c}{c_s} Kn \frac{H}{\delta x},
$$
 (48)

\nwhere l_o and l are the macroscopic property based mean free path and the local mean free path. For the gas flow between two parallel plates at $y = 0$ and $y = L$, the local mean free path of the molecules can be calculated as follows:

To consider the Knudsen layer effect, the local relaxation time should be determined, and can be related with the local mean free path as follows [24]:

$$
\tau = \frac{l}{l_o} \sqrt{\frac{\pi}{8}} \frac{c}{c_s} K n \frac{H}{\delta x},\qquad(48)
$$

 $\frac{1}{100}$ where l_o and *l* are the macroscopic property based mean free $\frac{200}{100}$ path and the local mean free path. For the gas flow between two parallel plates at $y = 0$ and $y = L$, the local mean free path of the molecules can be calculated as follows: $\alpha = \begin{cases}\n3/6 & \alpha = 0 \\
1/12 & \alpha = 1, 3, 5, 7 \\
1/16 & \alpha = 2, 4, 6, 8\n\end{cases}$ (47)
 $\alpha = 2, 4, 6, 8$ (47)
 $\alpha = 9, 10, 11, 12$
 $t_a = \begin{cases} 3/6 & a = 0 \\ 1/12 & a = 1, 3, 5, 7 \\ 1/16 & a = 2, 4, 6, 8 \end{cases}$ (47)

Il 16 $\alpha = 9, 10, 11, 12$

Fo consider the Knudsen layer effect, the local relaxation

as hould be determined, and can be related with the local

an f 1/12 $\alpha = 1, 3, 5, 7$ (47)

1/16 $\alpha = 1, 3, 5, 7$ (47)

1/16 $\alpha = 2, 4, 6, 8$ (17)

1/16 $\alpha = 9, 10, 11, 12$

onsider the Knudsen layer effect, the local relaxation

could be determined, and can be related with the local

$$
l(y) = l_o \left[1 + (\varphi - 1) \exp(-\varphi) - \varphi^2 \int_{\varphi}^{\infty} t^{-1} \exp(-t) dt \right],
$$
 (49)

where $\phi = y/l_o$ for the molecules moving towards $y = 0$ and $\phi =$ $(L-y)$ / l_o for moving towards $y = L$. The local mean free path of all molecules can be determined by averaging these two parts, because a molecule can move towards either side of the walls with equal probability. For $y = 0$ or $y = L$, $\phi = L/l_o$ can be used.

3.2 Boundary treatments

on in the shear rate along the walls. all molecules can be determined by averaging these two parts,

electity distribution in 3D gas micro-

because a molecule can move towards either side of the walls

one complicated th For the case of the combination of the wall equilibrium and the free-slip boundary conditions, only the information of the particle distribution function f_{10} needs to be added in the Eqs. (19)-(21). For high order LB method, therefore, the boundary condition at the lower wall is as follows: $\begin{aligned}\n\mathcal{L}(y) &= I_o \left[1 + (\varphi - 1) \exp(-\varphi) - \varphi^2 \right]_e^{\varphi} t^{-1} \exp(-t) dt \right],\n\end{aligned}$ (49) $\mathcal{L}(y) / I_o$ for moving towards $y = I_o$. The local mean free path of

molecules can be determined by averaging these two parts,
anse a mo sere $\phi = y/l_o$ for the molecules moving towards $y = 0$ and $\phi = y/l_o$ for moving towards $y = L$. The local mean free path of
molecules can be determined by averaging these two parts,
ause a molecule can move towards either si y/l_o for moving towards $y = L$. The local mean free path of
molecules can be determined by averaging these two parts,
ause a molecule can move towards either side of the walls
h equal probability. For $y = 0$ or $y = L$, $\$ ause a molecule can move towards either side of the walls
hequal probability. For $y = 0$ or $y = L$, $\phi = L/l_o$ can be used.
Boundary treatments
free-slip boundary conditions, only the information of the therefore,
differen

$$
f_2(x, y, t + \delta t) = \sigma f_2^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_8(x - \delta x, y + \delta x, t),
$$

(50)

$$
f_3(x, y, t + \delta t) = \sigma f_3^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_7(x, y + \delta x, t),
$$

(51)

$$
f_4(x, y, t + \delta t) = \sigma f_4^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_6(x + \delta x, y + \delta x, t),
$$

$$
(52)
$$

$$
f_{10}(x, y, t + \delta t) = \sigma f_{10}^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_{12}(x, y + 2\delta x, t).
$$
\n(53)

 $\alpha = 0$ momentum for re-emitted particles from the bottom wall as The other boundary condition can be derived in similar way of the standard LB method except the specular factor. The specular factor, *r*, should be recalculated from the sum of x $f_2(x, y, t + \delta t) = \sigma f_2^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_s(x - \delta x, y + \delta x, t)$,
 $f_3(x, y, t + \delta t) = \sigma f_3^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_7(x, y + \delta x, t)$,

(50)
 $f_4(x, y, t + \delta t) = \sigma f_4^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_6(x + \delta x, y + \delta x, t)$,
 $f_{10}(x, y, t + \delta t) = \sigma f_4^{eq}(\rho_w$ *x* $f_2(x, y, t + \delta t) = \sigma f_2^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_s(x - \delta x, y + \delta x, t)$,

(50)
 $f_3(x, y, t + \delta t) = \sigma f_3^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_7(x, y + \delta x, t)$,

(51)
 $f_4(x, y, t + \delta t) = \sigma f_4^{eq}(\rho_w, \vec{u}_w, t) + (1 - \sigma) f_6(x + \delta x, y + \delta x, t)$,
 $f_9(x, y, t + \delta t) = \sigma f$ x, y, t + δt) = $\sigma f_s^{eq}(P_w, \vec{u}_w, t) + (1 - \sigma) f_s(x - \delta x, y + \delta x, t)$,

(50)

x, y, t + δt) = $\sigma f_s^{eq}(P_w, \vec{u}_w, t) + (1 - \sigma) f_7(x, y + \delta x, t)$,

(51)

x, y, t + δt) = $\sigma f_s^{eq}(P_w, \vec{u}_w, t) + (1 - \sigma) f_6(x + \delta x, y + \delta x, t)$,

(52)

(52)

(

$$
J_x = f_2 - f_4 = (1 - 2r)(f_8 - f_6) = \frac{\rho}{4} u_w (1 - u_w) ,
$$
 (54)

Fig. 8. Non-dimensional velocity profiles for Poiseuille flow at *Kn* = 0.1128, 0.4514, and 0.9027.

Fig. 9. LB model comparison of nonlinearity of pressure and slip velocity distributions for $Kn_0 = 0.1$ and $\sigma = 0.9$.

$$
r = \frac{1}{2} - \frac{\rho}{8} \frac{u_w (1 - u_w)}{f_8 - f_6}.
$$
 (55) $\frac{c}{f}$

Thus, non-fully diffuse reflection can be possibly achieved by following boundary condition:

$$
f_2(x, y, t) = r \sigma f_6(x, y, t) + (1 - r \sigma) f_8(x, y, t) , \qquad (56)
$$

$$
f_3(x, y, t) = f_7(x, y, t),
$$
\n(57)

$$
f_4(x, y, t) = r \sigma f_8(x, y, t) + (1 - r \sigma) f_6(x, y, t) ,
$$
 (58)

$$
f_{10}(x, y, t) = f_{12}(x, y, t) \tag{59}
$$

3.3 Numerical simulation

For the comparison with the solution of the linearized

Boltzmann equation obtained by Ohwada et al. [25], the simulations of gas flows in an infinitely long microchannel are carried out. Fig. 8 shows the nondimensional velocity profiles for Poiseuille flow at $Kn = 0.1128$, 0.4514, and 0.9027. It is seen that the accurate results that are close to the direct solution of the Boltzmann equation can be obtained by high order LB method with the present boundary conditions. The results for σ = 0.8 are also presented in the figure.

f x, y, i + $\frac{1}{255}$ *b* $\frac{1}{255}$ *x x* (*x*) $\frac{1}{255}$ *x* (*x*) $\frac{1}{255}$ *x* (*x*) $\frac{1}{255}$ *x* (*x*) *x*) *x* (*x*) *x* (*x*) *x* (*x*) *x* To examine the Knudsen layer effect on the slip velocity, the long microchannel gas flows are simulated. The grid size for *H* is restricted to 30 δx (32 points), and L/H = 80 is used as for the standard case. P_i/P_o is set to 2.0. Fig. 9 shows the nonlinearity of the pressure and the slip velocity along the stream direction for $Kn_o = 0.1$ and $\sigma = 0.9$. When compared with the solutions obtained by the standard LB method, it is observed that the nonlinearity of the pressure increases, and the slip velocity along the wall decreases when the Knudsen layer

(a) Nonlinearity of pressure normalized by the outlet pressure (b) Slip velocity normalized by the outlet centerline velocity

Fig. 10. Nonlinearity of pressure and slip velocity distributions for $Kn_0 = 0.4$ and $\sigma = 0.9$.

Fig. 11. Non-dimensional the dynamic velocity profiles for $Kn = 0.4$ and $S = 1.0$.

effect is considered. In Fig. 10, the results of $Kn_0 = 0.4$ and σ = 0.9 are plotted. As the Knudsen number increases, the nonlinearity of the pressure decreases, and the slip velocity gets larger.

Finally, oscillatory Couette flow is also calculated to find out whether the present boundary conditions are available for transitional flow with a moving wall. Fig. 11(a) compares the dynamic velocity profiles for $Kn = 0.4$ and $S = 1.0$ from the high order LB method with present boundary conditions reflection, free-slip boundary condition is used, and the wall against the DSMC data [20]. It is seen that the velocity profiles are in excellent agreement with DSMC results even in the Knudsen layer. In Fig. 11(b), the results for σ = 0.9 are illustrated to see the tangential moment accommodation coefficient effect.

4. Conclusions

In this study, rarefied gas flows are simulated in the slip and the transition flow regime. In the simulations, the effect of the TMAC is considered. For the boundary treatment of non-fully diffuse wall, two new boundary conditions, which achieve the non-fully diffuse reflection by a linear combination of the diffuse and specular reflection, are proposed. For the specular equilibrium and specular bounce-back schemes are used for the diffuse reflection. The TMAC, σ , weighs the fraction of diffusive reflection and specular reflection. For the slip flow simulations, 2D/3D microchannel flows and oscillatory sheardriven gas flow are considered, and the results are in excellent agreement with the analytic solutions. To investigate the Knudsen layer effect, high order LB method is applied, and the present boundary conditions are slightly modified. It is found out that present boundary treatments are also applicable for the simulations of transition flow.

Nomenclature-

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