Journal of Southeast University (English Edition) Vol. 35, No. 1, pp. 30 - 35 Mar. 2019 ISSN 1003—7985

Multi-relaxation-time lattice Boltzmann simulation of slide damping in micro-scale shear-driven rarefied gas flow

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Abstract: To investigate the slide film damping in the micro-scale shear-driven rarefied gas flows, an effective multi-relaxation-time lattice Boltzmann method (MRT-LBM) is proposed. Through the Knudsen boundary layer model, the effects of wall and rarefaction are considered in the correction of relaxation time. The results of gas velocity distributions are compared among the MRT, Monte Carlo model (DSMC) and high-order LBM, and the effects of the tangential momentum accommodation coefficient on the gas velocity distributions are also compared between the MRT and the high-order LBM. It is indicated that the amendatory MRT-LBM can unlock the dilemma of simulation of micro-scale non-equilibrium. Finally, the effects of the Knudsen number, the Stokes number, and the gap between the plates on the damping are researched. The results show that by decreasing the Knudsen number or increasing the Stokes number, the slide film damping increases in the transition regime; however, as the size of the gap increases, the slide film damping decreases substantially.

Key words: lattice Boltzmann method; multi-relaxation-time; slide film damping; shear-driven oscillating flow

DOI: 10.3969/j. issn. 1003 - 7985. 2019. 01. 005

The modern technologies associated with microstructures such as micro-electro-mechanical systems, fuel cells and biochips have attracted significant interest recently and there is an urgent need for thorough research of physical phenomena and mechanisms of microstructures[1]. However, due to the complexities of the flow characteristics and the rarefaction effects in the transition and free-molecular-flow regimes, an accurate evaluation of the slide film damping in the micro-scale Couette plate flow is still a challenging issue. The rarefaction effects are described by the Knudsen number Kn, and the mean free path of molecules λ divided by the feature length L. We will simulate the oscillating Couette flow in the transition flow regime.

Received 2018-09-23, **Revised** 2019-01-11.

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Foundation item: The National Natural Science Foundation of China (No. 51375091).

Citation: Song Xucheng, Li Pu, Zhu Rui. Multi-relaxation-time lattice Boltzmann simulation of slide damping in micro-scale shear-driven rarefied gas flow[J]. Journal of Southeast University (English Edition), 2019, 35(1): 30 - 35. DOI: 10.3969/j. issn. 1003 - 7985. 2019. 01. 005.

The microscale flow has been studied in several works[2-3]. The corrected Reynolds equation is a common theoretical model applied to the micro-scale rarefied flow, which is commonly solved by a numerical approach, such as the Monte Carlo model (DSMC). Although the DSMC method has made great progress in simulating the rarefied gas flow with high Knudsen number, statistical noise will be generated when we evaluate the micro-scale flow damping at a low velocity, and thereby, the calculation costs are excessively high[4]. The molecular dynamics (MD) will be more suitable for the simulation of the liquid or dense gas flow; however, the application of the MD for simulating the rarefied gas flow and the micro-scale flow is not recommended due to the large amount of calculation and the slow convergence[5]. In the Lattice Boltzmann equation, the nonlinearity is imbedded in the left-hand side and the nonlinear advection is replaced by the linear streaming process. Therefore, it is different from macroscopic methods, which need to solve the Poisson equation at each time step to satisfy the continuous equation, and this fact greatly reduces the calculation time[6]. In addition, the collision and streaming processes are local, so the LBM method can be easily implemented in parallel computing, which further shortens the computational time.

Based on the mesoscopic scale, the precision of the lattice Boltzmann model (LBM), which can simulate the micro-scale flow and address these challenges, is compared to the DSMC or the direct solution methods. Furthermore, the LBM methodology has a good computational stability, and the boundary conditions can be easily handled, which is appropriate for parallel computing. The series of achievements have been acquired in simulating the microfluidic systems by employing LBM in the past few decades. The work by Nie at al. [7] is among the first ones that employed the LBM in simulating the microchannel flow as well as explaining the boundary slip velocity. However, the boundary adopted a nonslip bounce back scheme and the slip velocity was later confirmed as a discrete error [8]. Subsequently, Succi. [9] combined the rebound with the specular-reflection to characterize the slip velocities of the solid boundaries. After introducing the discrete diffuse boundary condition by Ansumali and Karlin[10], Tang et al. [11] established a general discrete form of the diffuse reflection. Meng et al. [12] systematically discussed the problems of the physical symmetry and the relaxation time selection in the gas micro-flow.

Owing to the inability of the standard LBM to capture the boundary Knudsen layer, some of its deficiencies have been revealed by conducting further research on the mechanics of the gas flow in the transition regimes. When the thin gas flows through the wall, a Knudsen layer that concerns the mean free path of molecules λ forms above the wall, in which the collision between the molecules is not sufficient and the molecule thermal equilibrium assumption would be no longer valid[13]. For solving these problems, the higher-order LBM was adopted by adding the higher-order equilibrium distribution function as well as the high precision Gauss-Hermite integral. However, introducing the high-order moment increases the complexity of the model, and the storage and computation costs increase, so some inherent advantages of the LBM will be limited. In this paper, a corrected effective relaxation time LBM is proposed, which takes into account the collision effect between the molecules and wall by introducing effective relaxation time. Furthermore, the MRT-LBM method can effectively reduce the problems of the increasing number of calculations and the storage produced by using the higher-order LBM method for simulating the gas flow in the transition regimes or a large Kn.

The above-mentioned literature mostly displays the simulations of the steady-state micro-scale flow; however, the engineering applications frequently involve the non-equilibrium gas flow such as micro-accelerometers, inertial sensors, resonant filters, and so on. As a result, a new numerical algorithm is required to evaluate the damping forces caused by the non-equilibrium effect of the gas flow. Tang et at.[14] employed a higher-order LBM to model the unsteady gas flow problems of the micro-scale single plate oscillation Couette flow. On this basis, we adopt the MRT-LBM to simulate the single plate periodic oscillating Couette flow on a micro-scale, and try to verify the correctness of the LBM in the analysis of the non-equilibrium micro-scale gas flow as well as the driven plate slide damping.

1 Micro-Scale Gas Flow LBM

1.1 MRT-LBM

In the momentum space, the collision operator can be expressed as

$$\boldsymbol{f}(x+c\Delta t, t+\Delta t)-\boldsymbol{f}(x,t)=-\boldsymbol{G}^{-1}\boldsymbol{S}[\boldsymbol{g}(x,t)-\boldsymbol{g}^{\mathrm{eq}}(x,t)] \tag{1}$$

where $\boldsymbol{g}(x,t)$ and $\boldsymbol{g}^{\mathrm{eq}}$ are the vectors of moments; $\boldsymbol{f}$ is the velocity distribution function; $\boldsymbol{S}$ is the relaxation matrix, and $\boldsymbol{G}$ is the transformation matrix.

The conversion between the speed and the moment space can be achieved by the following linear transformation:

$$\boldsymbol{g}=\boldsymbol{G}\boldsymbol{f} \tag{2}$$

$$\boldsymbol{f}=\boldsymbol{G}^{-1}\boldsymbol{g} \tag{3}$$

The discrete velocities c_k of D2Q9 is given by

$$\boldsymbol{c}_k=\begin{cases}[0,0] & k=0\\ a\cos(k-1)\pi/4 & k=1,2,3,4\\ \sqrt{2}\,a\cos(k-1)\pi/4 & k=5,6,7,8\end{cases} \tag{4}$$

where a is the lattice velocity and it is set to be 1 usually.

The matrix $\boldsymbol{G}$ for D2Q9 is shown as

$$\boldsymbol{G}=\begin{bmatrix}1&1&1&1&1&1&1&1&1\\-4&-1&-1&-1&-1&2&2&2&2\\4&-2&-2&-2&-2&1&1&1&1\\0&1&0&-1&0&1&-1&-1&1\\0&-2&0&2&0&1&-1&-1&1\\0&0&1&0&-1&1&1&-1&-1\\0&0&-2&0&2&1&1&-1&-1\\0&1&-1&1&-1&0&0&0&0\\0&0&0&0&0&1&-1&1&-1\end{bmatrix}$$

The moment vector $\boldsymbol{g}$ is $(\rho, w, \varepsilon, i_x, t_x, i_y, t_y, h_{xx}, h_{xy})^{\mathrm{T}}$, in which ρ is the density, and i_x and i_y are the x and y components of momentum.

$$i_x=\rho u_x=\sum_k f_k^{\mathrm{eq}}c_{kx} \tag{5}$$

$$i_y=\rho u_y=\sum_k f_k^{\mathrm{eq}}c_{ky} \tag{6}$$

Furthermore, the diagonal matrix $\boldsymbol{S}$ is

$$\boldsymbol{S}=\mathrm{diag}(0,0,1.4,0,s_1,0,s_1,s_2,s_2) \tag{7}$$

where s_1 and s_2 are the relaxation times.

The macro variables, including the density ρ, the fluid velocity vector $\boldsymbol{u}$, and the pressure p, are stated by

$$\rho=\sum_0^8 f_k \tag{8}$$

$$\boldsymbol{u}=\frac{1}{\rho}\sum_0^8 \boldsymbol{c}_k f_k \tag{9}$$

$$p=\rho c_s^2 \tag{10}$$

1.2 Boundary condition

The relaxation time s_2 associated with λ in the MRT-LBM is given as[13]

$$s_2=0.5+\frac{H}{\delta_x}Kn\sqrt{\frac{6}{\pi}} \tag{11}$$

where H is the gap between the plates.

However, when the thin gas flows through the wall, a Knudsen layer forms above the wall and in the transition regimes. It implies that the Knudsen layer is an essential factor in studying the micro-scale rarefied Couette flow. Therefore, we introduce the effective relaxation time model proposed by Guo[15], as follows:

$$s_2=0.5+\frac{H}{\delta_x}Kn\psi(y,Kn)\sqrt{\frac{6}{\pi}} \tag{12}$$

The modified function Ψ is

$$\Psi(y, Kn) = \frac{Z(y/\lambda) + Z(H - y/\lambda)}{2}$$
$$Z(\chi) = 1 + (\chi - 1)e^{-\chi} - \chi^2 T_n(\chi) \tag{13}$$

where

$$T_n(\chi) = \int_1^{\infty} t^{-1} e^{-\chi t} dt \tag{14}$$

in which $T_n(\chi)$ is the exponential integral function.

At the boundary walls, the slip velocity has a significant influence on the velocity distribution between plates and therefore, we adopt the boundary conditions of BSR proposed by Succi[9] and the wall is located at 1/2 the lattice sites. The three unknown distribution functions at the upper boundary with known velocity are

$$f_4 = f_2$$
$$f_7 = rf_5 + (1 - r)f_6 + \frac{2r\rho\omega_i \boldsymbol{c}_5 \cdot \boldsymbol{u}_w}{2c_s^2} \tag{15}$$
$$f_8 = rf_6 + (1 - r)f_5 + \frac{2r\rho\omega_i \boldsymbol{c}_8 \cdot \boldsymbol{u}_w}{2c_s^2}$$

where $\boldsymbol{u}_w$ is the upper plate velocity and r is the tangential momentum accommodation coefficient. For achieving the above-mentioned second-order slide boundary condition, the tangential momentum accommodation coefficient r and the relaxation time s_1 are given as

$$r = \left[1 + \zeta A_1 + \frac{\tau_s(H)\delta_x}{8\tau_q^2(H)}\right]^{-1} \tag{16}$$

$$s_1 = \left[0.5 + \frac{3 + 24\zeta^2\tau_q^2(H)A_2}{16\tau_q(H)} + \frac{\tau_s(H)\delta_x B}{16\tau_q(H)}\right] \tag{17}$$

where

$$\zeta = \sqrt{\frac{6}{\pi}} \tag{18}$$
$$\tau_q = s_2 - 0.5 \tag{19}$$
$$\tau_s = \frac{d\tau_s}{dy} \tag{20}$$
$$A_1 = \frac{2 - \sigma}{\sigma(1 - 0.1817\sigma)} \tag{21}$$
$$A_2 = \frac{1}{\pi} + 0.5 \times \frac{1}{A_1^2} \tag{22}$$
$$B = 12 + 30\tau_q(H)\zeta A_1 \tag{23}$$

2 Plate Oscillation Couette Flow

The upper surface at $z = d$ oscillates with velocity u_o along the horizontal direction, while the substrate has been fixed, as shown in Fig. 1. Two control parameters of the Couette flow are Kn and Stokes' number β, where the latter represents the relative relationship between the unsteady and the viscous effects, defined by

$$\beta = \sqrt{\frac{\omega L^2}{\upsilon}} \tag{24}$$

where υ is the kinetic viscosity; ω is the oscillatory frequency. The characteristics of the structure are listed in Tab. 1.

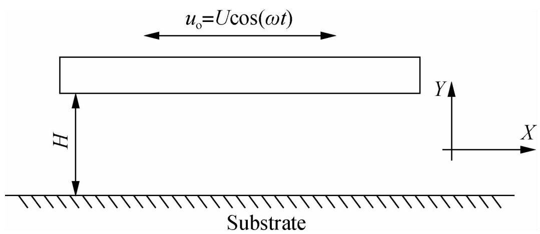

Fig. 1 The slide film damping of the Couette flow model

Tab. 1 Characteristics of the structure

Parameter	Value
Mass M/μg	0.26
Stiffness K/(N · μm^{-1})	3.8×10^{-7}
Structure thickness h/μm	1.8
Air-film thickness underneath the plate h_t/μm	2
Top surface of the plate A/μm^2	2.93×10^4
The kinetic viscosity υ_k/(μm^2 · s^{-1})	1.5×10^7
The maximum amplitudes U/μm	11

In LBM simulations, the correlation parameters are dimensionless and the mapping between physical units and lattice units can be performed by dimensionless criterion numbers. The mapping is shown in Tab. 2. Concerning the boundary conditions, the up and bottom adopt BSR and the left and right exploit periodic boundary conditions.

Tab. 2 Dimensionless lattice units for plate oscillation Coquette flow

Parameter	Physical symbol	Physical value	Lattice symbol	Lattice value
Sound speed/(μm · s^{-1})	c_t	3.404×10^8	c_s	$\sqrt{2}$
Heigh/μm	L_k	2	L_Y	8
Grid step/μm	Δx_o	0.2	Δx	1
Time step/μm	Δt_o	0.415	Δt	1
Kinematic viscosity/(μm^2 · s^{-1})	υ_o	1.5×10^7	υ_k	0.156
The maximum speed of oscillation plate/(μm · s^{-1})	U_o	9.02×10^{10}	U_k	0.001 87

3 Simulation Results

Fig. 2 demonstrates the velocity profiles at the mid-section, normalized by the maximum velocity of the driven plate. The maximum relative errors between the results of the MRT-LBM and those of the DSMC are lower than 30.87%, 32.51%, 31.99%, respectively, in Figs. 2 (a), (b) and (c). The maximum relative errors between the MRT-LBM and the high-LBM are lower than 23.94%, 18.11%, 23.45% in Figs. 2(a), (b) and (c).

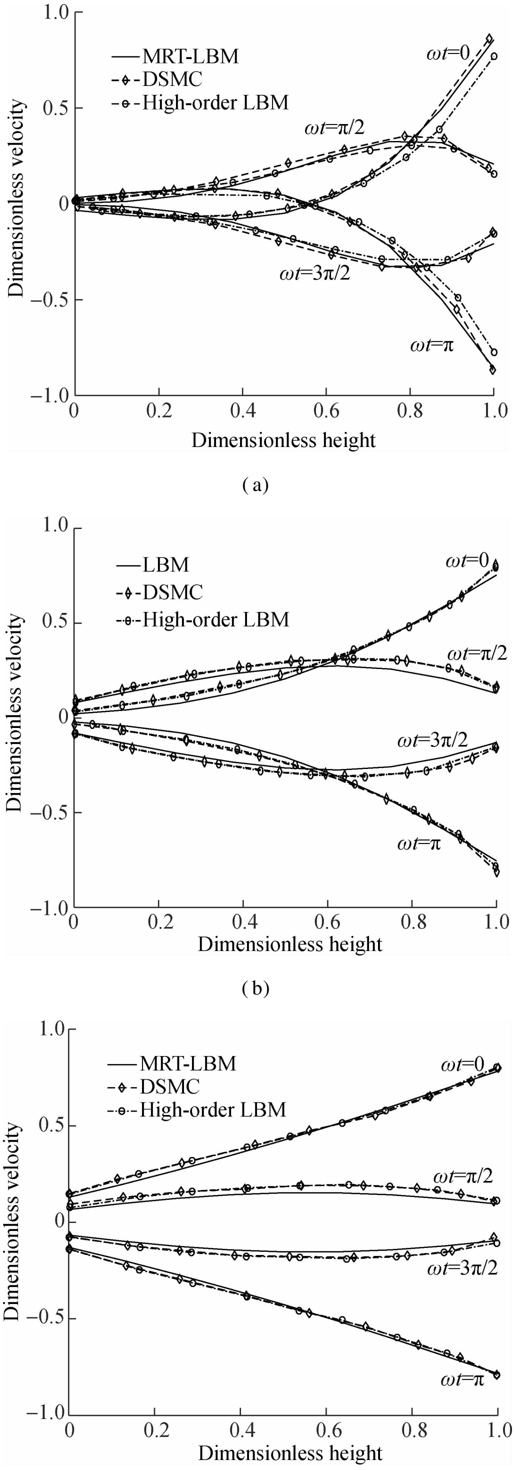

Fig. 2 Velocity profiles at the mid-section. (a) $Kn = 0.1$, $\beta = 4.0$; (b) $Kn = 0.2$, $\beta = 2.0$; (c) $Kn = 0.4$, $\beta = 1.0$

They indicate that the results acquired from the MRT-LBM are quite consistent with the DSMC data given by Hadjiconstantinou[16] as well as the high-LBM (D2Q13) data given by Tang et al[14].

Fig. 3 shows the velocity profiles of the mid-section ($L_X = 25$) at two moments during one cycle. The results of these profiles reveal that the slip velocity of the wall increases as the value of r decreases, which means that

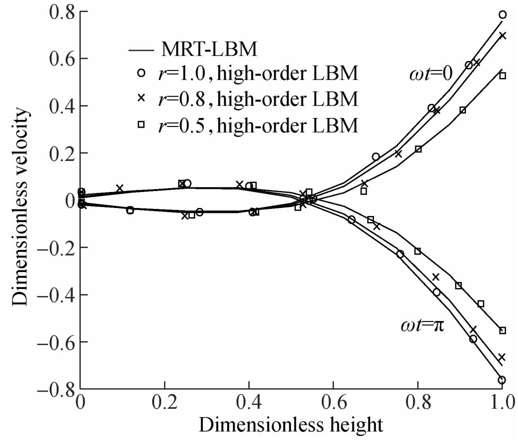

Fig. 3 Velocity profiles for $Kn = 0.1$, $\beta = 4.0$ revealing the effect of tangential momentum accommodation coefficient r

the slip film damping force is greater with a smaller value of r. The results are in good agreement with the high-order LBM data by Tang et al[14].

From the distribution function, the slide film damping can be evaluated directly. Therefore, it is convenient to compute the slide film damping and then compare it with that evaluated by the NS approaches. The predicted results of the slide film damping on the driven plate are shown in Fig. 4, which are normalized by the maximum value of the damping. When the Knudsen number is close to 0.1, the slide film damping increases obviously with the increase of the Stoke number. As the Knudsen number increases, the slide film damping decreases at the fixed Stokes numbers. The obtained findings are in a good agreement with the DSMC data by Hadjiconstantinou[16].

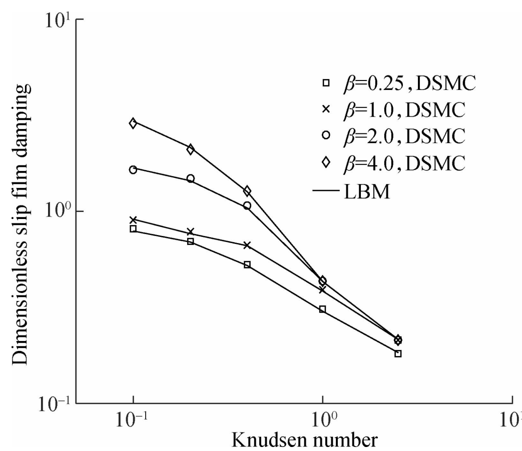

Fig. 4 Slide film damping on the driven plate with the Knudsen number

From the studies which display the velocity and damping profiles in terms of the Knudsen number or the Stokes number, we conclude that the MRT-LBM is reliable for simulating the non-equilibrium micro-scale gas flow and the driven plate slide damping. Therefore, the relationship between the slip film damping and the plate gap is explored as shown in Fig. 5. As the size of the gap increases, the slide film damping decreases obviously, so for the larger Knudsen numbers, the slide film damping is smaller.

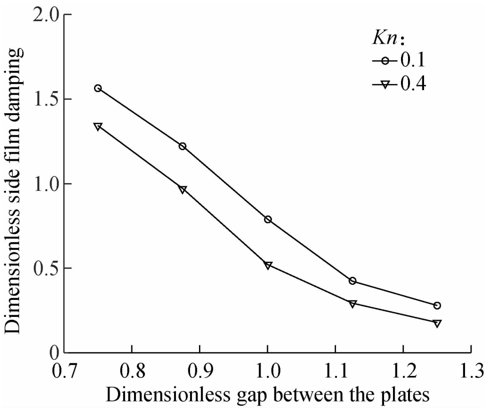

Fig. 5 Slide film damping on the driven plate as a function of the gap between plates

4 Conclusions

1) An effective MRT-LBM approach was presented to investigate the slide film damping in laterally driven microstructures by taking into account the Knudsen layer. The velocity distributions between the driven plate and the substrate were examined, and the predicted results were in a good agreement with those of the DSMC.

2) The connections between the slide film damping on the driven plate and the Knudsen number, the Stokes number, and the gap between plates were investigated. The researchers found that slide film damping will increase, particularly in the transition regime, by decreasing the Knudsen number, size of gaps or increasing the Stokes number.

3) In contrast to the DSMC method, the proposed MRT-LBM gives a better slide film damping evaluation. Furthermore, the obtained results confirm the importance of considering the Knudsen layer in non-equilibrium flow simulations.

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微尺度剪切驱动流滑移膜阻尼的有效多松弛时间格子 Boltzmann 模拟

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摘要: 采用 Knudsen 边界层模型将壁面效应与稀薄效应引入松弛时间的修正中,通过修正后的有效多松弛时间-格子 Boltzmann 模型(MRT-LBM)进一步研究微尺度剪切驱动流滑移膜阻尼的物理特性. 对比 MRT-LBM 模型与蒙特卡洛模型、高阶格子 Boltzmann 模型的板间速度分布的吻合度;将切向动量调节系数 r 对板间速度分布的影响与高阶格子 Boltzmann 模型的数据进行分析对比,验证了 MRT-LBM 模型用于分析微尺度非平衡剪切驱动流滑移膜阻尼时的有效性. 最后利用该模型研究努森数 Kn、斯托克斯数 β 和板间间隙对微尺度剪切驱动流滑移膜阻尼的影响. 结果表明:在过渡区,对于平板剪切振荡驱动流,随着努森数或板间间隙的增大,上平板下表面的滑移膜阻尼逐渐减小;斯托克斯数越大,滑移膜阻尼越大.

关键词: 格子 Boltzmann 模型(LBM); 多松弛时间; 滑移膜阻尼; 剪切驱动振荡流

中图分类号: O354