



A New Relaxation Time Model for Lattice Boltzmann Simulation of Nano Couette Flows in Wide Range of Flow Regimes

S. Ghatreh Samani and A. H. Meghdadi Isfahani [†]

Department of Mechanical Engineering, Najafabad branch, Islamic Azad University, Najafabad, Iran
Modern Manufacturing Technologies Research Center, Najafabad branch, Islamic Azad University,
Najafabad, Iran

[†]Corresponding Author Email: amir_meghdadi@pmc.iaun.ac.ir

(Received September 6, 2018; accepted February 17, 2019)

ABSTRACT

The standard LBM with the relaxation time is only able to simulate the flow features in continuum and slip regimes. In the present paper, a new relaxation time formulation considering the rarefaction effect on the viscosity for the lattice Boltzmann simulation of shear driven flows is presented in order to cover wide range of the flow regimes. The results show that in spite of the standard Lattice Boltzmann Method, LBM, the presented relaxation time equation is able to predict flow features in wide range of flow regimes including slip, transition and to some extent free molecular flow regimes. The velocity profiles, slip length and shear stress agree very well with DSMC (Direct Simulation Monte Carlo) and linear Boltzmann results.

Keywords: Lattice Boltzmann method; Micro and nano- Couette; Transitional regime; Knudsen number; Relaxation time; Rarefaction.

NOMENCLATURE

Kn	Knudsen number	μ_{eff}	effective viscosity
C_f	skin friction coefficient	σ_v	tangential momentum accommodation
C_{f0}	skin friction coefficient in no slip flows	τ_{cont}	shear stress in continuum regime
f	particle distribution function	τ_{∞}	shear stress in free molecular regime
f_i^{eq}	equilibrium distribution function	τ_f	relaxation time
h	height	τ_{eff}	effective relaxation time
Q	flow rate	τ_w	shear stress on the wall
R	gas constant	l_s	slip length
T_w	wall temperature	μ_0	dynamic viscosity
U	velocity	ρ	density
λ	mean free path	ν	kinematic viscosity

1. INTRODUCTION

Given the extensive applications of MEMS and NEMS (Micro and Nano Electro Mechanical Systems) in industries, flow and heat transport in micro/nano-instruments have attracted much scientific attention in today's world (Nguyen & Wereley, 2006). Flow behavior in micro/nano-geometries is different from that in macro-geometries. The very small dimensions of these instruments induce a quality, known as rarefaction, in the fluids they are interacting with.

This quality is expressed by the dimensionless Knudsen number, which is the ratio of mean free path, λ , to characteristic length, l , ($Kn=\lambda/l$) (Gad-el-Hak, 2001). Experimental investigation of dynamic and thermal properties of the flow in micro-channels leads to specific intervals for different flow regimes based on Knudsen number (Li *et al.* 2018a, Liu *et al.* 2018). For $Kn<0.001$, the fluid is continuous and Navier-Stokes equations are valid. But for $Kn>10$, $0.1<Kn<10$ or $0.001<Kn<0.1$, free molecular, transient and slip flow regimes are assumed respectively. Often,

heat transfer and flow in slip regimes are considered as micro-flows (Xie *et al.* 2018, Ho *et al.* 1998). These regimes can take place in any subtle flow. They are to be investigated by particle-based methods such as Molecular Dynamics, MD, (Bird, 1994) or Direct Simulation Monte Carlo, DSMC, (Oran *et al.* 1998) methods. The high computational cost and complex mathematical equations incorporated in MD and DSMC methods (Kandlikar *et al.* 2005) have made researchers to pursuit better methods, such as the Lattice Boltzmann Method, LBM, for simulating macro- and micro-flows (Chen *et al.* 1998; Li *et al.* 2018b; Ma *et al.* 2018).

Given their extensive applications in electronics, energy engineering, bio-technology, ... micro- and nano-Couette flows are a couple of the most general subjects of study in many fields of science and engineering, with their modeling being very important in science and industrial applications. Air flow between the sheets of computer hard discs, high-rpm centrifugal pumps and some micro- and nano-pumps can be mentioned as a few examples of their applications (Karniadakis *et al.* 2005). The oil film in rotating equipment such as cylinders and pistons with micrometer gaps are examples of micro-Couette flow. Engineering applications for this type of flow include: Couette flow mixers, rotary separator filters, bearings, catalytic chemical reactors and liquid-liquid separators (Karniadakis *et al.* 2005).

Modeling and analyzing gas flow in thin ducts such as micro- and nano-channels requires knowledge of nano-science. Experimental measurement is extremely hard at this scale and is associated with a considerable error. Measuring tools must be smaller than the geometries at this scale. Therefore, precision numerical modeling of these tools is of great importance. Precision numerical modeling can provide the capability for designing such equipment by identifying the flow field and its characteristics of performance. Considering the difficulty of preparing costly laboratory equipment, methods for analyzing flow at micro-scale seem to be crucial. An efficient and precise method for flow modeling is the lattice Boltzmann method. This method is based on tracking particles of the fluid using the Boltzmann equation. Lattice Boltzmann method incorporates lattice, equilibrium distribution functions and kinetic equation which is known as the lattice Boltzmann equation. Analysis of the flow field with complex boundaries, simple programming rules and easy conditions for parallel-processing are some advantages of using this method (Basha *et al.* 2018; Wu *et al.* 2018 ; Chen *et al.* 2010; Al-Zoubi *et al.* 2008). In this method, virtual particles move on a regular lattice and collide, and then the probability for these particles to be present in different paths is used.

Moreover the Lattice Boltzmann Equation (LBE) is a more fundamental equation compared to the Navier Stokes equations, which is valid for all ranges of flow regimes (Gad-el-Hak, 1999). Therefore, the LBM can be used to simulate fluid

flows in all regimes upon appropriate adjustments (Sbragaglia, Succi 2005).

There have been several studies on simulation of Couette flow in transitional flow regime by linear Boltzmann equation (Sone, 1990), DSMC (Fan *et al.* 2003), and Burnett equation (Xue *et al.* 2001; Bao *et al.* 2007). Moreover, different studies have addressed Couette flow in the slip flow regime via the lattice Boltzmann method (Nie *et al.* 2002; Tang *et al.* 2004; Shirani & Jafari 2007; Ghazanfarian & Abbassi, 2010; Shamshiri *et al.* 2012; Guo *et al.* 2008; Yang *et al.* 2017), but there has been no effort made to simulate Couette flow in transitional and free molecular flow regimes by LBM.

The standard lattice Boltzmann method, corresponded relaxation time of $\tau_r = Kn.H$, is not able to model transitional and free molecular flow regimes. The reason is that this relaxation time, merely considers molecular collision while the collisions between walls and molecules become important as Knudsen number increases. On the other hand, using high-order lattice Boltzmann methods provides reasonable results only for fluid flows at moderate Knudsen numbers (Zhou *et al.* 2006).

In previous studies for pressure driven flows (Normohammadzadeh *et al.* 2010; Shokouhmand *et al.* 2011; Homayoon *et al.* 2011; Meghdadi Isfahani *et al.* 2016; Zhang *et al.* 2012; Liou *et al.* 2014; Younes & Omidvar, 2015), it was shown that, by improving relaxation time, the lattice Boltzmann method becomes capable of providing accurate results for pressure-driven flows in all flow regimes.

In the present study, by relating the viscosity to the local Kn, a novel relaxation time formula is presented in such a way that wide range of Kn Couette flow regimes can be simulated more accurately.

2. GOVERNING EQUATIONS

Gas flow between two parallel plates separated by a distance h is assumed. Top plate moves to the right with the velocity u_0 while the bottom plate is stationary. The momentum equation governing this flow is as follows (Karniadakis *et al.* 2005):

$$\frac{d^2 u}{dy^2} = 0 \quad (1)$$

Solving the eq. 1 for continuum regime with no slip boundary condition yields:

$$u(y) = (u_0 / h)y \quad (2)$$

By applying the velocity slip boundary conditions as follows:

$$u_s - u_w = \frac{2 - \sigma_v}{\sigma_v} C_1 Kn \left(\frac{\partial u}{\partial n} \right)_s \quad (3)$$

where n denotes the normal vector and u_s and u_w are

gas velocity on the wall and wall velocity, respectively, The dimensionless velocity distribution for the slip flow regime is obtained as follows (Karniadakis *et al.* 2005):

$$\frac{u}{u_0} = \frac{\frac{y}{h} + \frac{2-\sigma_v}{\sigma_v} Kn}{1 + 2\frac{2-\sigma_v}{\sigma_v} Kn} \quad (4)$$

where y is distance from the bottom wall, and σ_v is the tangential momentum accommodation coefficient, which is an empirical coefficient amounting to zero for specular reflection and 1 for diffuse reflection (Bahukudumbi *et al.* 2003).

Flow rate is obtained by:

$$Q = \int_0^h u dy \quad (5)$$

Using the velocity distribution (Eq.4) in Eq. 5, yields the following relation for volumetric flow rate (Karniadakis *et al.* 2005):

$$\frac{Q}{u_0 h} = 0.5 \quad (6)$$

The analytical solution above shows that flow rate is constantly 0.5 for the incompressible micro-Couette flow in slip regime (Karniadakis *et al.* 2005). The ratio of the skin friction coefficient for shear-driven slip flows and no-slip flows (C_f) is given by (Karniadakis *et al.* 2005):

$$\frac{C_f}{C_{f0}} = \frac{1}{1 + 2\frac{2-\sigma_v}{\sigma_v} Kn} \quad (7)$$

where $C_f = \tau_w / (1/2 \rho u_0^2)$, with τ_w the wall shear stress.

Previous results from DSMC and linearized Boltzmann methods show that the velocity distribution in Couette flow in the transition and free molecular flow regimes remain approximately linear. Therefore, second and higher degree derivatives are always zero, making it inadequate to apply second or higher degree boundary conditions. For this reason, researchers proposed different values for C_1 so it covers a wider range of flow regimes. For example, Marques *et al.* (2000) proposed $C_1=1.111$ and showed that where plates move with the velocity of $\pm u_0$, the following velocity distribution provides appropriate results for $Kn < 0.25$:

$$u(Y) = \frac{2u_0 Y}{1 + 2\frac{2-\sigma_v}{\sigma_v} C_1 \times Kn} \quad (8)$$

Bahukudumbi *et al.* (2003) proposed a modified slip coefficient for C_1 as follows:

$$C_1 = \beta_0 + \beta_1 \tan^{-1}(\beta_2 Kn^{\beta_3}) \quad (9)$$

where $\beta_0=1.2977$, $\beta_1=0.71851$, $\beta_2=-1.17488$ and $\beta_3=0.58642$ are empirical constants that are obtained by comparing the velocity profile, obtained by the linearized Boltzmann method (Sone *et al.* 1990), with that obtained from Eq. 8. They

showed that unlike the first-order model, using Eq. 9 matches the velocity profile in the bulk flow region for a wide range of Knudsen numbers, while this model fails to predict the velocity distribution in the Knudsen layer and consequently the shear stress near the walls. This is expected, since the model is based on the Navier–Stokes equations, which is not valid for the transition and free molecular regimes.

3. LATTICE BOLTZMANN METHOD

Unlike other common numerical methods which are based on discretization of macroscopic continuum equations, the Boltzmann method is based on microscopic models and macroscopic kinetic equations.

The 9-speed 2-dimensional lattice Boltzmann method (D2Q9) is used for this study (Fig 1).

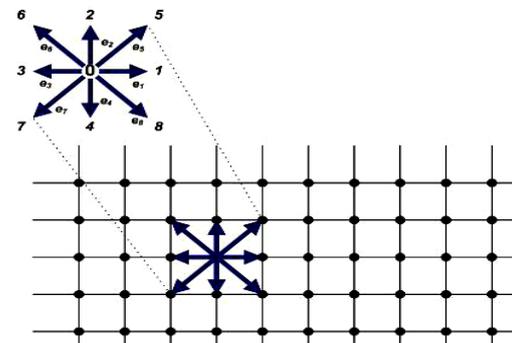


Fig. 1. D2Q9 lattice Boltzmann model.

Using the BGK collision operator (Bhatnagar *et al.* 1954), the discretized Boltzmann equation is:

$$f_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) - f_i(\vec{x}, t) = -\frac{1}{\tau_f + 0.5} [f_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)] \quad (10)$$

where f_i is the particle distribution function, τ_f is the dimensionless relaxation time and f_i^{eq} is the equilibrium distribution function:

$$f_i^{eq}(\vec{x}, t) = w_i \rho \left[1 + \frac{3\vec{c}_i \cdot \vec{u}}{c^2} + \frac{9(\vec{c}_i \cdot \vec{u})^2}{2c^4} - \frac{3(u^2 + v^2)}{2c^2} \right] \quad (11)$$

$$w_0 = \frac{4}{9} \quad w_{i=1,2,3,4} = \frac{1}{9} \quad w_{i=5,6,7,8} = \frac{1}{36}$$

where $c = \Delta x / \Delta t$ represents the base velocity on the lattice. Δx and Δt are lattice spacing and time step, respectively. The discrete velocity vector C_i in D2Q9 lattice is shown in Eq. 12.

$$c_i = \begin{cases} 0 & i = 0 \\ \left(\cos\left[\frac{(i-1)\pi}{4}\right], \sin\left[\frac{(i-1)\pi}{4}\right] \right) & i = 1, 2, 3, 4 \\ \sqrt{2} \left(\cos\left[\frac{(i-1)\pi}{4}\right], \sin\left[\frac{(i-1)\pi}{4}\right] \right) & i = 5, 6, 7, 8 \end{cases} \quad (12)$$

In discrete momentum space, local mass density ρ

and local velocity u are calculated by Eqs. 13 and 14.

$$\rho = \sum_i \bar{f}_i \quad (13)$$

$$\rho \bar{u} = \sum_i \bar{c}_i \bar{f}_i \quad (14)$$

Eq. 10 simulates collisions between particles in the flow. In this method, virtual fluid particles are assumed on lattice nodes with streaming and collision steps taking place on them. This equation includes two steps: collision (Eq. 15) and streaming (Eq. 16) as follows:

$$f_i^*(x, t) = f_i(x, t) - \frac{1}{\tau_f + 0.5} [f_i(x, t) - f_i^{eq}(x, t)] \quad (15)$$

$$f_i(x + c_i \Delta t, t + \Delta t) = f_i^*(x, t) \quad (16)$$

3.1 Boundary Conditions for Lattice Boltzmann Method

Periodic boundary conditions are assumed at inlet and outlet of the channel. In continuum regime, the bounce-back boundary condition is used to simulate no-slip condition on stationary walls, while, for the first time, a new boundary condition is proposed assuming no-slip conditions for moving walls. Moreover, the Diffuse Scattering Boundary Condition (DSBC) (Bhattacharya *et al.* 1989) is used to predict the slip velocity on solid walls.

3.2 No-Slip Boundary Condition for Moving Walls

Considering that velocity is known and constant on the top wall, a no slip boundary condition based on Zou and He method (Zou & He 1997) is developed to simulate moving wall at continuum flow regime. As shown in Fig 2, for the top wall, f_4 , f_7 and f_8 distribution functions and ρ are unknown. Four equations are needed in order to calculate the unknowns, while three can be obtained from momentum equations:

$$\rho = \sum f_i \Rightarrow f_4 + f_7 + f_8 = \rho_0 - (f_0 + f_1 + f_2 + f_3 + f_5 + f_6) \quad (17)$$

$$x: \rho u_x = f_1 - f_3 + f_5 - f_6 - f_7 + f_8 \Rightarrow f_8 - f_7 = \rho u_0 - f_1 + f_3 - f_5 + f_6 \quad (18)$$

$$y: \rho u_y = f_2 - f_4 + f_5 + f_6 - f_7 - f_8 \Rightarrow f_4 + f_7 + f_8 = f_2 + f_5 + f_6 \quad (19)$$

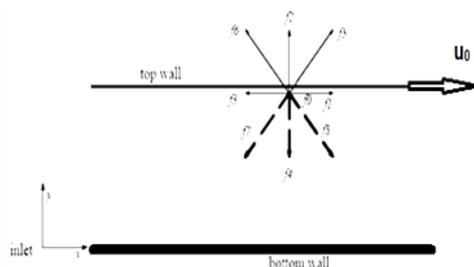


Fig. 2. Schematic of boundary conditions.

Another equation is needed for calculating the unknowns. The fourth equation can be written by assuming that the bounceback condition holds in the direction normal to the boundary as proposed by Zou and He (Zou & He 1997).

$$f_2 - f_2^{(eq)} = f_4 - f_4^{(eq)} \quad (20)$$

This is a system of four equations with four unknowns, and it can be solved as follows:

$$f_4 = f_2$$

$$f_8 = f_6 + \frac{1}{2}(f_3 - f_1) + \frac{\rho_0 u_0}{2} \quad (21)$$

$$f_7 = f_5 - \frac{1}{2}(f_3 - f_1) - \frac{\rho_0 u_0}{2}$$

$$\rho_0 = f_0 + f_1 + f_3 + 2(f_2 + f_5 + f_6)$$

3.3 New Relaxation Time Relation for wide Range of Knudsen Numbers

The shear stress for Couette flows exhibits two distinct behaviors in the continuum and free-molecular flow regimes (Bahukudumbi *et al.* 2003). In the continuum flow regime the shear stress for Couette flows is proportional to the velocity gradient as given by:

$$\tau_{cont} = \mu_0 \frac{du}{dy} \quad (22)$$

where the viscosity is $\mu_0 = \sqrt{2RT_w} / \pi \rho \lambda$, while in the free molecular flow regime the shear stress is proportional to the relative velocity of plates (Kogan, 1969):

$$\tau_\infty = -\rho U \sqrt{2RT_w} / \pi \quad (23)$$

Bahukudumbi *et al.* (2003) presented an analytical expression for the shear stress using different molecular interaction models, i.e.

$$\pi_{xy} = \frac{\tau}{\tau_\infty} = \frac{aKn^2 + 2bKn}{aKn^2 + cKn + b} \quad (24)$$

where π_{xy} is the shear stress in the entire Knudsen regime normalized with the free molecular shear stress and the coefficients $a=0.5297$, $b=0.6030$, and $c=1.6277$ are obtained by a least squares fit to the linearized Boltzmann solution (Sone *et al.* 1990). Using the new velocity slip model of Eq. 9 and the shear stress model given by Eq. 24 a generalized diffusion coefficient named as “effective viscosity” is defined:

$$\mu_{eff} = \frac{\mu_0}{2} \frac{aKn + 2b}{aKn^2 + cKn + b} (1 + 2C_1 Kn) \quad (25)$$

where μ_0 is the dynamic viscosity of the gas at continuum flow regime. It should be noted that viscosity at continuum flow regime differs from viscosity at transition and free molecular flow regimes. The dynamic viscosity at continuum flow regime is related to the diffusion of momentum due to the intermolecular collisions only, while for the

transition regime, because of the rarefaction, intermolecular collisions and molecule-wall collisions have the same order and in the free molecular regime, the molecule-wall collisions are the dominant phenomenon. Thus the effective diffusion coefficient, μ_{eff} , is presented in order to consider the intermolecular collisions and molecule-wall collisions.

For D_2Q_9 model, kinetic viscosity is related to relaxation time as follows:

$$\nu = \tau_f RT \Rightarrow D_2Q_9: RT = 1/3 \Rightarrow \nu_{eff} = \frac{\tau_{eff}}{3} \quad (26)$$

where ν , R and T are kinematic viscosity, gas constant and temperature in lattice unites. For D_2Q_9 model $RT=1/3$ in lattice unites.

Substituting Eq. 25 into Eq. 26, yields:

$$\tau_{eff} = \frac{3\mu_{eff}}{\rho} = \frac{3}{2} \frac{\mu_0}{\rho} \frac{aKn + 2b}{aKn^2 + cKn + b} (1 + 2C_1Kn) \quad (27)$$

For the standard LBM with $\tau_f = Kn H$ (H is the number of lattice across the characteristic length of the flow domain) viscosity is related to the relaxation time as follow:

$$\mu_0 = \frac{1}{3} \rho \cdot \tau_f = \frac{1}{3} \rho Kn H \quad (28)$$

Hence:

$$\tau_{eff} = \frac{3\mu_{eff}}{\rho} = \frac{KnH}{2} \frac{aKn + 2b}{aKn^2 + cKn + b} (1 + 2C_1Kn) \quad (29)$$

Eq. 29 shows the relation between effective relaxation time of lattice Boltzmann with Knudsen number. Applying this relation to the codes, the capability of lattice Boltzmann method in modeling micro- and nano-Couette flows in transient and free molecular regimes is enhanced. The standard lattice Boltzmann method uses the relaxation time $\tau_f = Kn H$ which is only applicable at small Knudsen numbers, while τ_{eff} is applicable for wide range of Knudsen numbers (except $Kn=0$) covering continuum, slip, transition and free molecular flow regimes because it is derived from effective viscosity which considers the molecule-wall collisions in addition to the intermolecular collisions.

4. RESULTS

In order to simulate flow in continuum and slip regimes, a Couette flow with fixed bottom plate and moving top plate ($u_0=0.1$ m/s) is considered while for transient and free molecular regimes a Couette flow with two plates moving in opposite directions at the velocity U (Fig 3) is assumed.

Three grid sizes are considered: 160×60 , 320×120 and 640×240 . The results of using the aforementioned grids are compared in Figs 4 and 5 for slip ($Kn=0.05$) and free molecular ($Kn=10$) regimes respectively. The 320×120 grid is found to be appropriate.

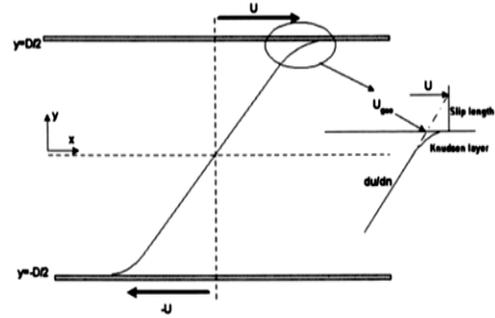


Fig. 3. Schematic view of linear Couette flow and the corresponding velocity profile for rarefied gas flows.

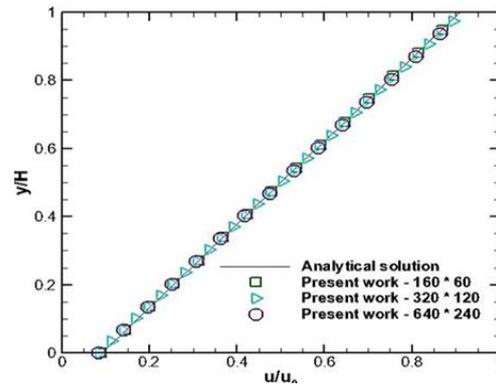


Fig. 4. Grid independency for $Kn=0.05$.

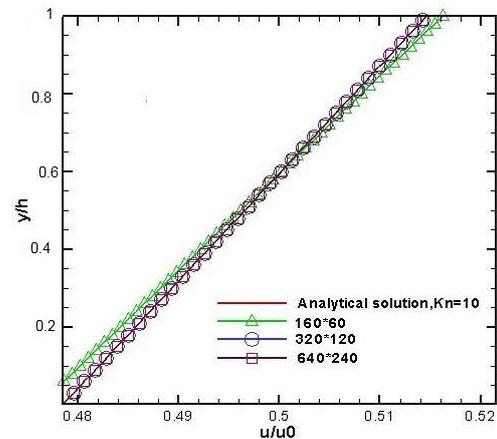


Fig. 5. Grid independency for $Kn=10$.

To validate the results, fig 6, compares the normalized volumetric flow rate along the micro-channel obtained by the standard LBM ($\tau_f = KnH$) and new model (Eq. 29) with those of the analytical approach of Eq. 6. All three methods show the constant value 0.5.

Fig 7 shows the c_i/c_{i0} ratio along the micro-channel obtained from standard LBM and new model, assuming $\sigma_v=1$ and $Kn=0.05$. Analytical results of Eq. 7 are also presented. It is evident from the figure that analytical and numerical solutions are in good agreement, showing the accuracy of the

results. Furthermore, it can be concluded that for low Kn in continuum and slip regimes, new model and standard LBM have the same results.

Because Eq. 29 is not valid for $Kn=0$, $Kn=0.001$ with no-slip boundary condition is considered to calculate C_{f0} for continuum flow regime.

Velocity distributions across the channel are plotted in Figs 8 and 9 for $Kn=0.001$ and $Kn=0.01$ respectively using the new relation time (Eq. 29). The results pertaining to analytical solution of Eq.2 and those of standard relaxation time $\tau_r=KnH$ are also presented. Comparison shows that the proposed relaxation time model is capable of modeling velocity distribution in continuum and slip regimes.

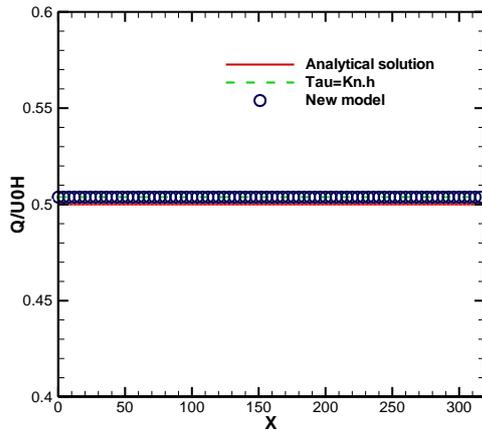


Fig. 6. Normalized volumetric flow rate along the micro/nano channel $Kn=0.05$.

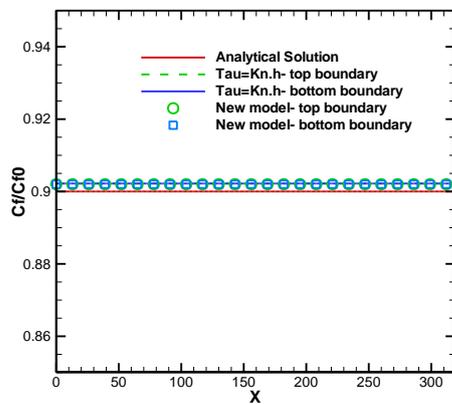


Fig. 7. Normalized skin friction coefficient along the microchannel for $Kn = 0.05$.

Fig 10 shows the velocity distributions obtained from the new model for $Kn=0.001, 0.01, 0.1, 0.5$. The corresponding results of standard LBM and analytical results of Eq. 8 are also included. The results show good agreement, however for $Kn=0.5$, a little discrepancy can be seen between the results of Eq. 8 and LBM results because Eq. 8 is accurate for $Kn<0.25$. It can be seen from the figure that the results of the proposed model are similar to those of the standard lattice Boltzmann in slip regime. It is evident that all velocity profiles are linear in the new model and slip velocity increases on the walls

of the micro-channel as Knudsen number increases, leading to larger slip length. Intersection of all diagrams is located at the center of the micro-channel due to the symmetry of slip velocity.

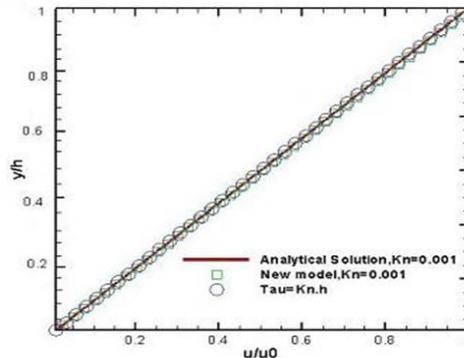


Fig. 8. Velocity distribution obtained from new models, analytical results and Standard lattice Boltzmann ($\tau_r=KnH$) for $Kn=0.001$.

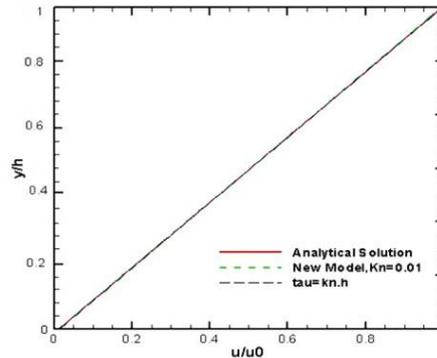


Fig. 9. Velocity distribution obtained from new models, analytical results and Standard lattice Boltzmann ($\tau_r=KnH$) for $Kn=0.01$.

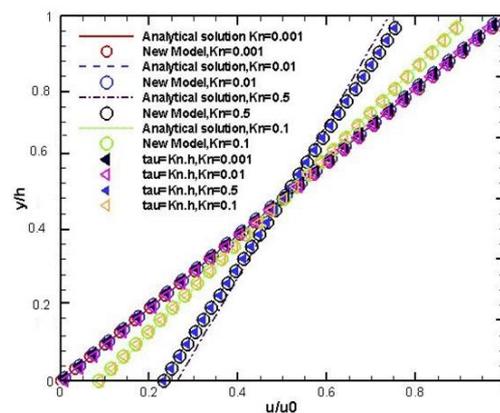


Fig. 10. Velocity distribution obtained from new models, analytical results and Standard lattice Boltzmann ($\tau_r=KnH$) for $Kn=0.001, 0.01, 0.1, 0.5$.

In Figs. 11, 12 and 13 velocity profiles in the upper half of the channel obtained from the new relaxation time relation (Eq. 29) are compared with those of obtained by linear Boltzmann equation

(Sone *et al.* 1990), DSMC (Bahukudumbi *et al.* 2003), analytical results of Navier Stokes equations using first order slip velocity (Ohwada *et al.* 1998) and the analytical solution of Eq.8, for $K=0.1$, $K=1$ and $K=10$ respectively, where $K = \frac{\sqrt{\pi}}{2} Kn$.

By increasing Knudsen number, the results of standard LBM ($\tau=KnH$) deviate from the results of DSMC and linear Boltzmann methods while, the presented results by new model are accurately compatible with linearized Boltzmann and DSMC methods in the entire transition flow regime.

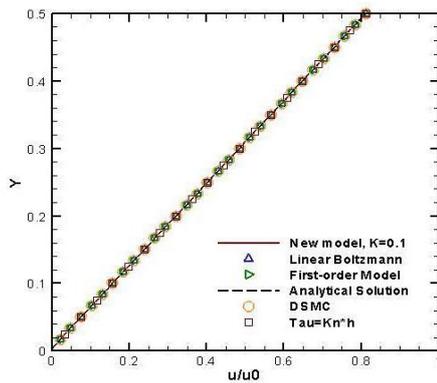


Fig. 11. Velocity distributions obtained from new model, analytical results (Marques *et al.* 2000), Standard LBM, linear Boltzmann (Sone *et al.* 1990) and DSMC (Bahukudumbi *et al.* 2003) for $K=0.1$.

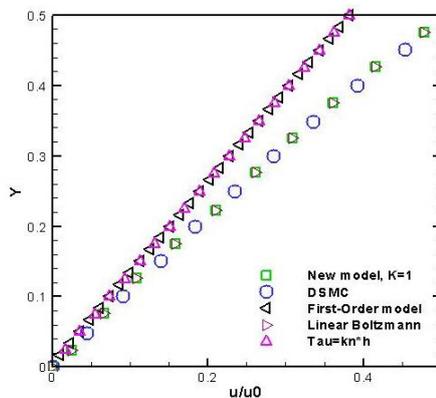


Fig. 12. Velocity distributions obtained from new model, analytical results (Marques *et al.* 2000), Standard LBM, linear Boltzmann (Sone *et al.* 1990) and DSMC (Bahukudumbi *et al.* 2003) for $K=1$.

It is concluded from Figs 12 and 13 that the results of standard LBM perfectly match those of the Navier Stokes equations with first order slip velocity (Ohwada *et al.* 1998) for all Knudsen numbers. In fact these methods are Equivalent.

Fig. 14 shows the velocity distribution in the upper-half of the channel for $K= 0.1, 1$ and 10 . It is evident that the velocity profiles in the transition flow regime remain linear. The velocity decreases

as Knudsen number increases which is also expected from the analytical solution according to Eq. 8.

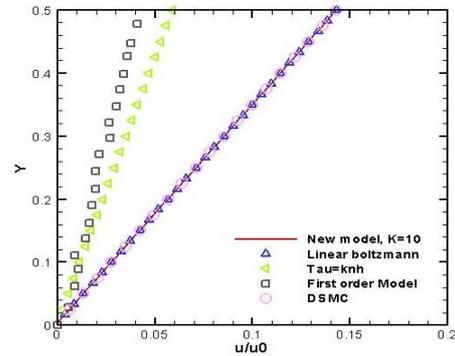


Fig. 13. Velocity distributions obtained from new model, analytical results (Marques *et al.* 2000), Standard LBM, linear Boltzmann (Sone *et al.* 1990) and DSMC (Bahukudumbi *et al.* 2003) for $K=10$.

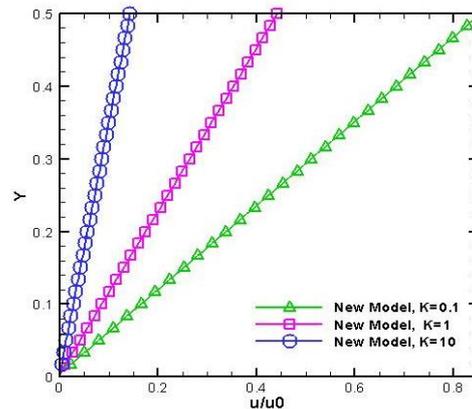


Fig. 14. Velocity profiles for upper-half of the channel at $K = 0.1, 1$, and 10 .

Slip Velocity is usually characterized by a non-dimensional parameter, known as the slip length (l_s), which is the distance from the solid wall, where the extrapolated bulk flow velocity is equal to the wall velocity. A no-slip boundary condition is equivalent to $l_s = 0$, whereas a slip boundary condition results in a finite slip length, $l_s > 0$. Bhattacharya & Lie (1989) and Morris *et al.* (1992) analyzed slip-length variation as a function of the Knudsen number using molecular dynamics and variable hard-sphere DSMC simulations. Following Bhattacharya & Lie (1989), the non-dimensional slip-length (l_s) can be written as follows:

$$l_s = \frac{u\left(y = \frac{D}{2}\right) - U}{D \frac{\partial u(y)}{\partial y}} \quad (30)$$

The velocity gradient $\partial u/\partial y$ is determined from the velocity profile outside the Knudsen layer, as illustrated in Fig 3. Slip velocity at the surface ($u(y = D/2)$) is obtained by extrapolating the bulk-flow

velocity profile to the wall.

Fig. 15 shows normalized slip length obtained from the presented new model of Eq. 29 as well as the standard lattice Boltzmann method ($\tau_r=KnH$) and DSMC (Bahukudumbi *et al.* 2003).

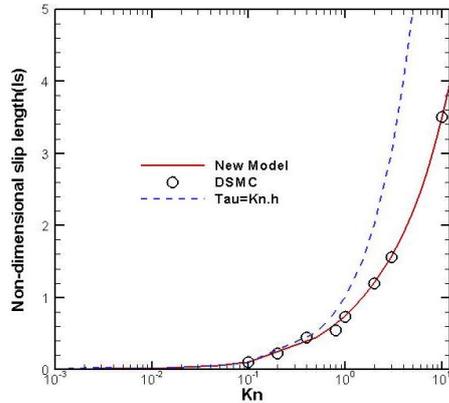


Fig. 15. Normalized slip length as a function of Knudsen number.

It is seen that the slip length calculated by using the proposed model is in a good agreement with those of DSMC in the wide range of Knudsen numbers while the standard relaxation time can only works well at Knudsen number less than 1; This fact indicates the inability of the standard model and at the same time it implies the suitable ability of the new presented correlation. It should be noted that this success is achieved with no changes in the boundary conditions.

In Fig. 16 shear stress normalized by the corresponding continuum value is plotted as a function of Knudsen number. Because Eq. 29 is not valid for $Kn=0$ The continuum shear stress is calculated by $\tau_{xy}=\mu_{eff} du/dy$ for $Kn=0.001$ with no-slip boundary condition. It is evident from Fig 18 that the results of the proposed model are in good agreement with those of DSMC (Bahukudumbi *et al.* 2003) and linear Boltzmann method (Sone *et al.* 1990) which implies the suitable performance of the proposed model for shear stress of micro-Couette flow in wide range of Knudsen numbers.

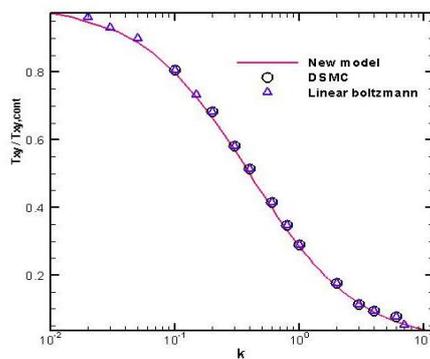


Fig. 16. Variation of normalized shear stress with modified Knudsen number K.

5. CONCLUSION

The standard LBM with the relaxation time $\tau_r=KnH$ is only able to simulate the flow features in continuum and slip regimes. In this paper a new relaxation time relation for lattice Boltzmann simulation of nano Couette flows is proposed. The new LBM is capable of simulating the flow for a wide range of Knudsen numbers including the transition and to some extent free molecular regimes. It is shown that the proposed model is able to predict the flow features in micro and nano scales for wide range of Kn, accurately. In slip flow regime the results of standard LBM and new model are identical. Non-dimensional velocity distribution, slip length and shear stress are in good agreement with available numerical data for wide range of Knudsen numbers. These results are obtained without incorporating any kind of adjustable slip models.

REFERENCES

- Al-Zoubi, A. and G. Brenner (2008). Simulating fluid flow over sinusoidal surfaces using the lattice Boltzmann method. *Computers and Mathematics with Applications* 55, 1365-1376.
- Bahukudumbi, P., J. H. Park and A. Beskok (2003). A unified engineering model for steady and quasi-steady shear-driven gas micro flows. *Journal of Micro scales Thermo physical Engineering* 7 (4), 291-315.
- Bao, F. B., J. Z. Lin and X. Shi (2007). Burnett simulation of flow and heat transfer in micro Couette flow using second-order slip conditions. *International Journal of Heat and Mass Transfer* 43 (6), 559-566.
- Basha, M. and N. A. C. Sidik (2018). Numerical predictions of laminar and turbulent forced convection: Lattice Boltzmann simulations using parallel libraries. *International Journal of Heat and Mass Transfer* 116, 715-724.
- Bhatnagar, P. L., E. P. Gross and M. A. Krook (1954). Model for collision process in gases. I. Small amplitude processes in charged and neutral one-component system. *Physics Review* 94, 511.
- Bhattacharya, D. K. and G. C. Lie (1989) Molecular-dynamics simulations of nonequilibrium heat and momentum transport in very dilute gases. *Physical Review Letters* 62, 897-900.
- Bird, G. (1994). *Molecular gas dynamics and the direct simulation of gas flows*, Oxford University Press.
- Chen, S. and G. D. Doolen (1998). Lattice Boltzmann method for fluid flows. *Annual Review of Fluid Mechanics* 30, 329-364.
- Chen, S. and Z. Tian (2010). Entropy generation analysis of thermal micro-Couette flows in slip regime. *International Journal of Thermal*

- Sciences* 49, 2211-2221.
- Fan, J. and C. Shen (2001). Statistical simulation of low-speed rarefied gas flows. *Journal of Computational Physics* 167(2), 393-412.
- Gad-el-Hak, M. (1999). The fluid mechanics of microdevices *Journal of Fluids Engineering* 12 (1), 5-33.
- Gad-el-Hak, M. (2001). *Flow physics in MEMS. Mécanique and industries*, 2, 313-341.
- Ghazanfarian, J. and A. Abbassi (2010). Heat transfer and fluid flow in microchannels and nanochannels at high Knudsen number using thermal lattice-Boltzmann method. *Physical review E* 82, 026307.
- Guo, Z., C. Zheng and B. Shi (2008). Lattice Boltzmann equation with multiple effective relaxation times for gaseous microscale flow. *Physical review E* 77, 036707.
- Ho, C. and Y. Tai (1998). Micro-electro-mechanical-systems (MEMS) and fluid flows. *Annual Review of Fluid Mechanics* 30, 579-612.
- Homayoon, A., A. H. Meghdadi Isfahani, E. Shirani and M. Ashrafizadeh (2011). A novel modified lattice Boltzmann method for simulation of gas flows in wide range of Knudsen number. *International Journal of Communications in Heat and Mass Transfer* 38 (6), 827-832.
- Kandlikar, S., S. Garimella, D. Li, S. Colin and M.R. King (2005). *Heat transfer and fluid flow in minichannels and microchannels*. Elsevier.
- Karniadakis, G., A. Beskok and N. Aluru (2005). *Microflows and nanoflows fundamentals and simulation*, Springer Inc., USA.
- Kogan, M. N. (1969). *Rarefied Gas Dynamics*, Plenum Press, New York.
- Li, S., Q. Li, S. Fu and K. Xu (2018a). A unified gas-kinetic scheme for axisymmetric flow in all Knudsen number regimes. *Journal of Computational Physics* 366, 144-169.
- Li, X., J. Fan, H. Yu, Y. Zhu and H. Wu (2018b). Lattice Boltzmann method simulations about shale gas flow in contracting nano-channels. *International Journal of Heat and Mass Transfer* 122, 1210-1221.
- Liou, T. M. and C. T. Lin (2014). Study on microchannel flows with a sudden contraction-expansion at a wide range of Knudsen number using lattice Boltzmann method. *Microfluidics and nanofluidics* 16(1), 315-327.
- Liu, W., G. Tang, W. Su, L. Wu and Y. Zhang (2018). Rarefaction throttling effect: Influence of the bend in micro-channel gaseous flow. *Physics of Fluids* 30, 082002.
- Ma, N., Z. Duan, H. Ma, L. Su, P. Liang, X. Ning, B. He, X. Zhang (2018). Lattice Boltzmann Simulation of the Hydrodynamic Entrance Region of Rectangular Microchannels in the Slip Regime. *Micromachines* 9 (2), 87.
- Marques, W., G. M. Kremer and F. M. Sharipov (2000). Couette flow with slip and jump boundary conditions. *Continuum Mechanics and Thermodynamics* 12, 379-386.
- Meghdadi Isfahani, A. H., I. Tasdighi, A. Karimipour, E. Shirani and M. Afrand (2016). A joint lattice Boltzmann and molecular dynamics investigation for thermohydraulic simulation of nano flows through porous media. *European Journal of Mechanics B/Fluids* 55, 15-23.
- Morris, D. L., L. Hannon and A. L. Garcia (1992). Slip length in a dilute gas. *Physical Review Letters* 46, 5279-5281.
- Nguyen, N. T. and S. T. Wereley (2006). *Fundamentals and applications of microfluidics*. Second edition, Artech house INC, Norwood.
- Nie, X., G. D. Doolen and S. Y. Chen (2002). Lattice Boltzmann simulation of fluid flows in MEMS. *Journal of Statistical Physics* 107, 279-289.
- Normohammadzadeh, M., M. M. Rahnama, S. Jafari and A. Akhgar (2010). Simulation of Long Microchannel Flow in Transitional Regime Using Lattice Boltzmann Method. *ASME 2010 8th International Conference on Nanochannels, Microchannels, and Minichannels collocated with 3rd Joint US-European Fluids Engineering Summer Meeting. American Society of Mechanical Engineers*.
- Ohwada, T., Y. Sone and K. Aoki (1998). Numerical analysis of the shear and thermal creep flows of a rarefied gas over a plane wall on the basis of the linearized Boltzmann equation for hard sphere molecules. *Physics of Fluids A* 1, 1588-1599.
- Oran, E. S., C. K. Oh, B. Z. Cybyk (1998). Direct Simulation Monte Carlo: Recent Advances and Applications. *Annual Review of Fluid Mechanics* 30 (1), 403-441.
- Sbragaglia, M. and S. Succi (2005). Analytical calculation of slip flow in lattice Boltzmann models with kinetic boundary conditions. *Physics of Fluids* 17, 093602.
- Shamshiri, M., M. Ashrafizaadeh and E. Shirani (2012). Investigation of flow and heat transfer characteristics of rarefied gaseous slip flow in nonplanar micro-Couette configuration. *International Journal of Thermal Sciences* 54, 262-275.
- Shirani, E. and S. Jafari (2007). Application of LBM in simulation of flow in simple micro-geometries and micro porous media. *The African Review of Physics* 1.0002.

- Shokouhmand, H. and A. H. Meghdadi Isfahani (2011). An improved thermal lattice Boltzmann model for rarefied gas flows in wide range of Knudsen number. *International Communications in Heat and Mass Transfer* 38, 1463–1469.
- Sone, Y., S. Takata and T. Ohwada (1990). Numerical analysis of the plane Couette flow of a rarefied gas on the basis of the linearized Boltzmann equation for hard-sphere molecules. *European Journal of Mechanics B Fluids* 9, 273-288.
- Tang, G.H., W.Q. Tao, Y.L. He (2004) Lattice Boltzmann method for simulation gas flow in micro channel. *International Journal of Modern Physics C*. 15, 335-347.
- Wu, S., C. Yu, F. Yu and Y. Chen (2018). Lattice Boltzmann simulation of co-existing boiling and condensation phase changes in a confined micro-space. *International Journal of Heat Mass Transfer* 126, 773–782.
- Xie, F., Y. Li, X. Wang, Y. Wang, G. Lei and K. Xing (2018). Numerical study on flow and heat transfer characteristics of low pressure gas in slip flow regime. *International Journal of Thermal Science* 124, 131-145.
- Xue, H., Ji, H. M., Shu, C., (2001). Analysis of micro-Couette flow using Burnett equations. *International Journal of Heat Mass Transfer* 44, 4139–4146.
- Yang, L. M., C. Shu, J. Wu, Y. Wang (2017). Comparative study of discrete velocity method and high-order lattice Boltzmann method for simulation of rarefied flows. *Computers and Fluids* 146, 125–142.
- Younes, B. and A. Omidvar (2015). Calculation of friction coefficient and analysis of fluid flow in a stepped micro-channel for wide range of Knudsen number using Lattice Boltzmann (MRT) method. *Physica A: Statistical Mechanics and its Applications* 440, 161-175.
- Zhang, W. M., G. Meng, and X. Wei (2012). A review on slip models for gas microflows. *Microfluidics and nanofluidics* 13 (6), 845-882.
- Zhou, Y., R. Zhang, I. Staroselsky, H. Chen, W. T. Kim and M. S. Jhon (2006). Simulation of micro- and nano-scale flows via the lattice Boltzmann method. *Physica A* 362, 68-77.
- Zou, Q. and X. He (1997). On pressure and velocity boundary conditions for the lattice Boltzmann BGK model. *Physics of Fluids* 9 (6), 1591-1598.