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Application of Lattice Boltzmann Method to Fluid Flows in Microgeometries

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Abstract

In the present investigation, Lattice Boltzmann Method (LBM) is used to simulate rarefied gaseous microflows in three microgeometries. These are micro-couette, micro lid-driven cavity and micro-poiseuille flows. The Knudsen number is used to measure the degree of rarefaction in the microflows. First, micro-couette flow is computed with the effects of varying Knudsen number in the slip and threshold of the transition regime and the results compare well with existing results. After having thus established the credibility of the code and the method including boundary conditions, LBM is then used to investigate the micro lid-driven cavity flow with various aspect ratios. Simulation of microflow not only requires an appropriate method, it also requires suitable boundary conditions to provide a well-posed problem and unique solution. In this work, LBM and three slip boundary conditions, namely, diffuse scattering boundary condition, specular reflection and a combination of bounce-back and specular reflection is used to predict the micro lid-driven cavity flow fields. Then the LBM simulation is extended to micro-poiseuille flow. The results are substantiated through comparison with existing results and it is felt that the present methodology is reasonable to be employed in analyzing the flow in micro-systems.

Keywords: Lattice Boltzmann Method; Knudsen Number; micro-couette flow; micro lid-driven cavity flow; micro-poiseuille flow.

1. Introduction

In the last two decades there has been significant progress in the development of Micro-electro-mechanical systems (MEMS) and Nano-electro-mechanical systems (NEMS) at the application and as well as at the simulation levels [1]. The study of gaseous flow in these micro and nano-devices has been an interesting and active topic of research in recent days. Micro-devices have attracted increasing attention due to their applications in various fields, such as medicine, environment control, office equipment, home appliances etc [1, 2]. It is necessary to understand and employ the physical laws governing the flow in these small-scale devices to design the devices effectively.

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Traditional numerical simulations relying on continuum approach and the Navier-Stokes equations break down at higher values of the Knudsen number (*Kn)*, which equals the ratio of the mean free path of the gas molecules λ to the characteristic length H of the flow system. The Knudsen number is used to measure the degree of rarefaction in the microflows. According to Knudsen number range, the state of a gaseous flow can be defined in four different regimes. First, the gaseous flow for $Kn < 0.001$ is termed as continuum regime and the Navier-Stokes equations with no-slip boundary conditions are only appropriate and valid in this regime. Next, the gaseous flow range for Knudsen number $0.001 < Kn < 0.1$ is termed slip regime and $0.1 < Kn < 10$ is termed transition regime. In these regimes, the Navier-Stokes equation loses validity and the molecules hitting a solid wall experience, what is known as, slip. For $Kn > 10$ the regime can be considered as free molecular flow. In the above regimes, it is known that as the Knudsen number increases the non-continuum effects such as slip flow and non-equilibrium (or) rarefaction effects emerge.

The micro-couette flow problem is one of the simplest benchmark problems in rarefied gas dynamics. This problem is commonly encountered in several MEMS-based applications, ranging from micro-motors, micro-accelerometers, comb mechanisms to the flying slider heads in computer hard drives [3]. It is known that micro-couette flow is shear-driven and the pressure does not change in the streamwise direction. Micro lid-driven cavity is another common example of a microfluidic system. Cavities, steps and cut-outs occur frequently in many engineering designs [4]. The micro lid-driven cavity flows are quite simple in geometry but they display almost all micro-fluid mechanical phenomena. Study of micro-poiseuille flow is also a popular benchmark problem and it is a common configuration in biomedical applications [5]. Particle based methods such as Molecular Dynamics (MD) and the Direct Simulation Monte Carlo (DSMC) has made some progress in the simulation of microflows. In the past few years, Lattice Boltzmann Method (LBM) emerged as an alternative and computationally efficient method to study the rarefied gaseous flows [6]. It is also known that the LBM is a simplified solver of the Boltzmann Equation on a discrete lattice. Therefore, the choice of using Lattice Boltzmann Method for microflow simulation is a good one owing to the fact that it is based on the Boltzmann equation which is valid for the whole range of the Knudsen number (*Kn*). The Lattice Boltzmann method has been studied extensively by many researchers for incompressible fluid flows with no-slip boundary conditions only [7].

Very few numerical studies are available in the literature for rarefied gaseous microflows [8-17]. First, Nie et al. [8] used the LBM with bounce-back boundary condition to simulate two-dimensional micro-channel and micro lid-driven cavity flows. They employed the LBM in the no-slip and slip regime, but it is known that the no-slip boundary conditions are generally unrealistic for slip and transition flows and it cannot capture the real microflow characteristics. Raabe [9] has written a review paper on LBM for micro and nano-scale fluid dynamics in materials science and engineering. Naris and Valougeorgis [10] described a comprehensive study of the lid-driven cavity problem over the whole range of Knudsen number regime using the discrete velocity method to solve the linearized Boltzmann equation. Mizzi et al. [11] presented the solutions of a micro lid-driven square cavity using Navier-Stokes-Fourier equations. Niu et al. [12] used diffuse scattering boundary condition to simulate isothermal two-dimensional microchannel flows. Darbandi et al. [13] simulated micro lid-driven cavity flow with various aspect ratios using finite volume element method. The present work is concerned with the application of Lattice Boltzmann Method (LBM) to compute gaseous flows in microgeometries. The paper is organized in four sections. In Section 2 some aspects of the LBM with governing equation and associated boundary conditions are discussed. Section 3 includes the results and discussions. Finally in Section 4 concluding remarks are made.

2. Numerical Method

2.1. Lattice Boltzmann Method

The lattice Boltzmann method is an alternative and computationally convenient method for the simulation of fluid flows which is quite distinctive from molecular dynamics method (MD) on the one hand and the methods based on the discretization of partial differential equations (finite difference method, finite volume method, finite element method, spectral method) on the other. The Lattice Boltzmann method (LBM) which can be linked to the Boltzmann equation in kinetic theory is formulated as [14]

$$f_i(\mathbf{x}+\boldsymbol{c_i}\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\tfrac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)\right) \tag{1}$$

Here f_i is the particle distribution function, $\boldsymbol{c_i}$ is the particle velocity along the ith direction, $f_i^{(eq)}(\mathbf{x},t)$ is the equilibrium distribution function at $\mathbf{x}$, t and τ is the time relaxation parameter. In an incompressible fluid flow the relaxation time is related with viscosity based on the continuum assumption. It is known that the reference length in microflows is very small, and the continuum assumption may not be valid. To simulate microscopic gaseous flows Lim *et al.* [14] relates the relaxation time τ to the Knudsen number Kn. This relation is given by

$$\tau = Kn\,(N_y - 1) \tag{2}$$

where N_y is the number of lattice nodes in y-direction. In the present work we take $N_y = 300$. The *D2Q9* square lattice used here has nine discrete velocities. In this lattice each node has eight neighbours connected by eight links. Particles residing on a node move to their nearest neighbours along these links in unit time step. The particle velocities are defined as

$$\begin{aligned} c_i &= 0, \quad i = 0 \\ c_i &= (\cos(\pi/4(i-1)), \sin(\pi/4(i-1))), \quad i = 1, 2, 3, 4 \\ c_i &= \sqrt{2}(\cos(\pi/4(i-1)), \sin(\pi/4(i-1))), \; i = 5, 6, 7, 8. \end{aligned} \tag{3}$$

In the nine-speed square lattice, a suitable equilibrium distribution function that has been proposed in [14]

$$\begin{aligned} f_i^{eq} &= \rho w_i \left[1 - \frac{3}{2}\boldsymbol{u}^2\right], \; i = 0 \\ f_i^{eq} &= \rho w_i \left[1 + 3(\boldsymbol{c_i}.\boldsymbol{u}) + 4.5\,(\boldsymbol{c_i}.\boldsymbol{u})^2 - 1.5\,\boldsymbol{u}^2\right], \; i = 1, 2, 3, 4 \\ f_i^{eq} &= \rho w_i \left[1 + 3(\boldsymbol{c_i}.\boldsymbol{u}) + 4.5\,(\boldsymbol{c_i}.\boldsymbol{u})^2 - 1.5\,\boldsymbol{u}^2\right], \; i = 5, 6, 7, 8 \end{aligned} \tag{4}$$

where the lattice weights are given by $w_0 = 4/9$, $w_1 = w_2 = w_3 = w_4 = 1/9$ and $w_5 = w_6 = w_7 = w_8 = 1/36$. The macroscopic quantities such as density ρ and momentum density $\rho\boldsymbol{u}$ are defined as velocity moments of the distribution function f_i as follows:

$$\rho = \sum_{i=0}^{N} f_i\,, \tag{5}$$

$$\rho\boldsymbol{u} = \sum_{i=0}^{N} f_i \boldsymbol{c_i}. \tag{6}$$

2.2. Boundary Conditions

Boundary conditions play a crucial role in micro-geometries [15-17]. On the micro-scale, the standard no-slip boundary condition used in hydrodynamics has to be replaced by a slip boundary condition. In the present work, we adopt three slip boundary conditions, namely; combination of bounce-back and specular reflection boundary condition, diffuse scattering boundary condition and specular reflection boundary condition on the stationary walls. Combination of bounce-back and specular boundary condition using the tangential momentum accommodation coefficient (TMAC) is used to simulate the slip boundary condition. For gaseous flow in micro-devices the TMAC (σ) can be expressed as

$$\sigma = \frac{M_i - M_r}{M_i - M_W} \tag{7}$$

where M is the tangential momentum of the molecules and the subscripts i, r, w refer to the incident, reflected and wall molecules respectively. In case, $\sigma = 0,$ the condition will be pure specular that represents pure slip. This pure slip condition is known as specular reflection boundary condition (SBC). For $\sigma = 1$, it is pure bounce-back that represents no-slip. Next, the diffuse scattering boundary condition (DSBC) which is derived from the gas-surface kinetic theory is written as [12,18]

$$\left|\left(\boldsymbol{e}_i - \boldsymbol{u}_w\right).\boldsymbol{n}\right| f_i = \sum_{\left(\mathbf{e}_{i'} - \mathbf{u}_W\right).\mathbf{n}<0} \left|\left(\boldsymbol{e}_{i'} - \boldsymbol{u}_W\right).\boldsymbol{n}\right| \Re_f\left(\boldsymbol{e}_{i'} \rightarrow \boldsymbol{e}_i\right) f_{i'} \tag{8}$$

with

$$\Re_f\left(\boldsymbol{e}_{i'} \rightarrow \boldsymbol{e}_i\right) = \frac{A_N}{\rho_w}\left(\left(\boldsymbol{e}_i - \boldsymbol{u}_W\right).\boldsymbol{n}\right) f_i^{eq}\Big|_{\boldsymbol{u}=\boldsymbol{u}_W} \tag{9}$$

where i' and i are directions of the incident and reflected particles, respectively, and A_N is a normalization coefficient and can be obtained by satisfying zero normal flux conditions on the walls. This normalization coefficient A_N which guarantees no normal flow through the wall can be written as

$$A_N = \rho_w \frac{\sum_i \left|\left(\boldsymbol{e}_i - \boldsymbol{u}_W\right).\boldsymbol{n}\right| f_i}{\left|\left(\boldsymbol{e}_i - \boldsymbol{u}_W\right).\boldsymbol{n}\right| f_i^{eq}\Big|_{\boldsymbol{u}=\boldsymbol{u}_W} \sum_i \left|\left(\boldsymbol{e}_{i'} - \boldsymbol{u}_W\right).\boldsymbol{n}\right| f_{i'}} \tag{10}$$

For the *D2Q9* model the expression for A_N simply reduces to 6 [12].

3. Results and Discussions

A lattice node resolution study is carried out using three lattice sizes composed of 250×250, 300×300 and 350×350 lattice arrangements. The numerical results are equivalent for the 300×300 and 350×350 lattice sizes. Therefore 300×300 lattice size is considered in all simulations in the present study.

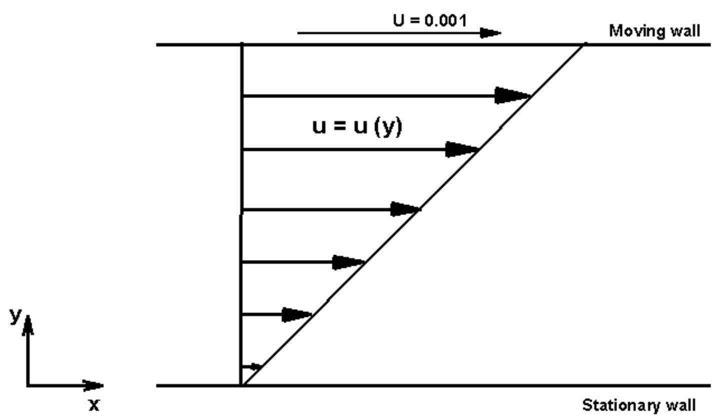


Figure 1. Geometry of a micro-couette flow.

3.1. Micro-couette flow

First, the developed LBM code is used to compute the micro-couette flow shown in Figure 1. In this problem the flow is confined between two parallel plates, and the upper plate moves with a constant velocity U and the lower plate is stationary. The flow field between the two plates is generated exclusively by the shear stress exerted on the fluid by the moving upper plate, resulting in a velocity profile across the flow $u = u(y)$, as sketched in Figure 1. Periodic boundary conditions are applied in the inlet and outlet. Initially the x-direction velocity is assumed to be uniform through out the channel except at the upper plate where the velocity is $U = 0.001$ and y-velocity is taken as 0. Density is initially set equal to 1.0. Combination of bounce-back and specular reflection boundary condition (BSBC) is used in the stationary wall ($\sigma = 0.7$). At moving (upper) wall particle distribution functions are updated by the equilibrium distribution function.

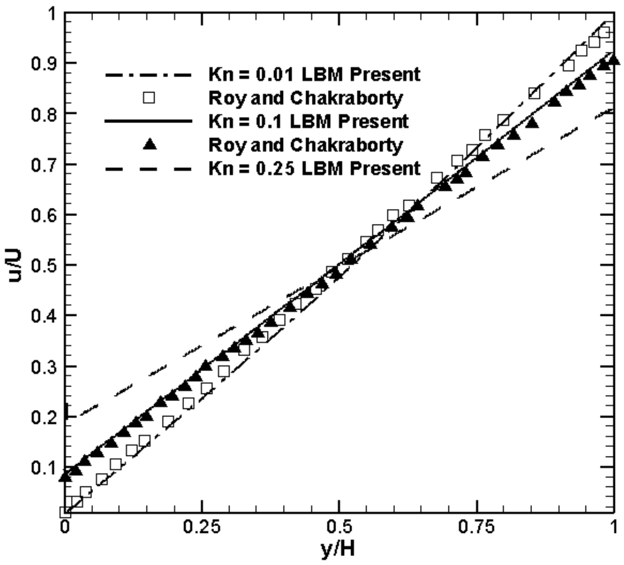


Figure 2. Micro-couette velocity profile for different *Kn.*

Figure 2 depicts the velocity profiles of gaseous flow between the plates for different Knudsen numbers (Kn = 0.01, 0.1 and 0.25). The predicted LBM results agree well with existing results of Roy and Chakraborty [3]. It is seen that as the Knudsen number increases, slip velocity at the walls increases, but the velocity profile remains linear and ‘symmetric’. Confirming of the results with existing results lends credibility to the present code and methodology, so that it is extended to the micro lid-driven cavity and micro-poiseuille flows in the next two subsections.

3.2. Micro lid-driven cavity flow

Here Lattice Boltzmann Method with *D2Q9* model is used to simulate the two-dimensional micro lid-driven cavity flows. As shown in Figure 3, in the micro-cavity the upper wall moves with a constant velocity U from the left to right and the other three walls remain stationary. The equilibrium distribution function is assigned to the particle distribution function at the surface of the moving wall. First, LBM is used to compute the micro-lid-driven cavity flow in a square cavity on a 300×300 lattice arrangement. From our study of the micro-couette flow we observe that a TMAC of $\sigma = 0.7$ produces results that are in good agreement with existing results. That is why on the stationary walls we use a combination of specular and bounce-back boundary condition using a TMAC of $\sigma = 0.7$. Figure 4 show for various Knudsen numbers, the *x*-velocity (*u*) profile along the vertical centreline and the *y*-velocity (*v*) profile along a horizontal centreline passing through the geometric centre of the cavity. These figures represent the effect of Knudsen number on the velocity profiles and on the velocity-slip condition at the boundary.

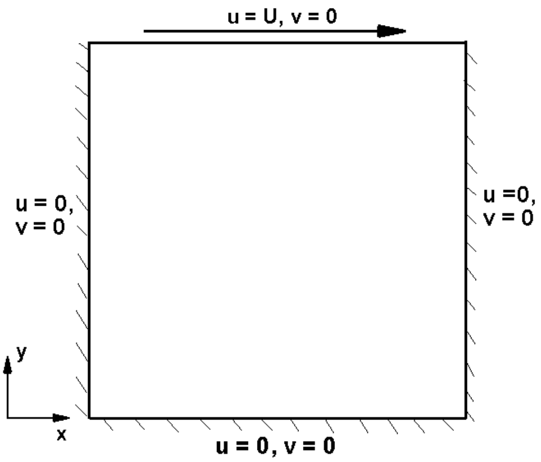
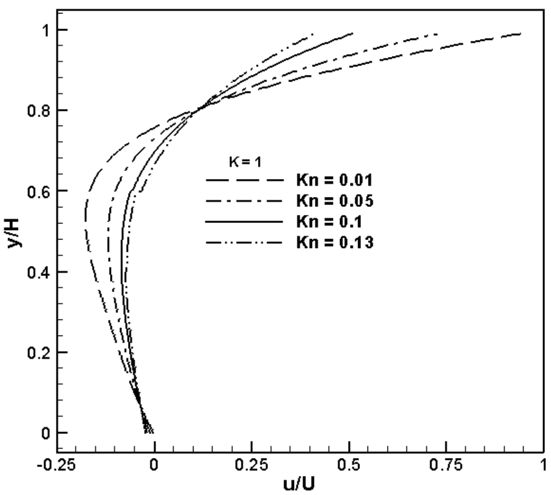
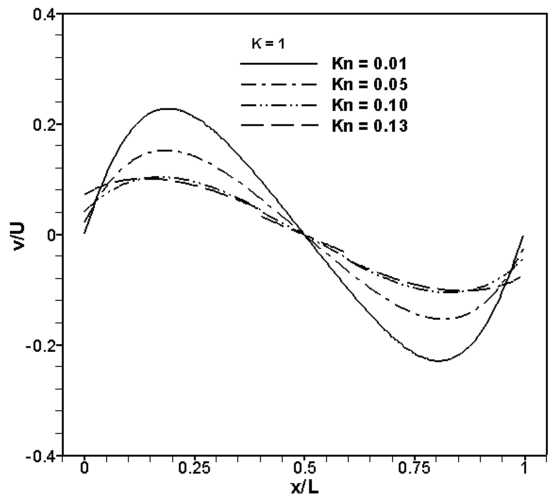


Figure 3. Geometry of a micro lid-driven cavity flow.

Figure 5 depicts the velocity profiles in the micro-lid-driven square-cavity flow for *Kn* = 0.05 with different boundary conditions, namely, BSBC ($\sigma = 0.7$), SBC and DSBC on the stationary walls. It is seen that BSBC and SBC velocity profile results are similar and DSBC result shows some deviation from these two slip boundary conditions. The reason may be that the DSBC is a slip boundary condition derived from gas-surface interaction law of the kinetic theory. Figure 6 depicts the streamline patterns for micro lid-driven cavity flow at *Kn* = 0.01 with aspect ratios *K* = 0.5, 2.0 and 5.0. For aspect ratio *K* = 0.5 and 1.0 there is only one primary vortex and for *K* = 2.0 and 5.0 secondary vortices appear under the top one and it is seen that as the aspect ratio of the cavity increases, the number of counter-rotating vortices appear at the bottom increases. It is also seen that, the flow is almost symmetric with respect to the vertical centreline.

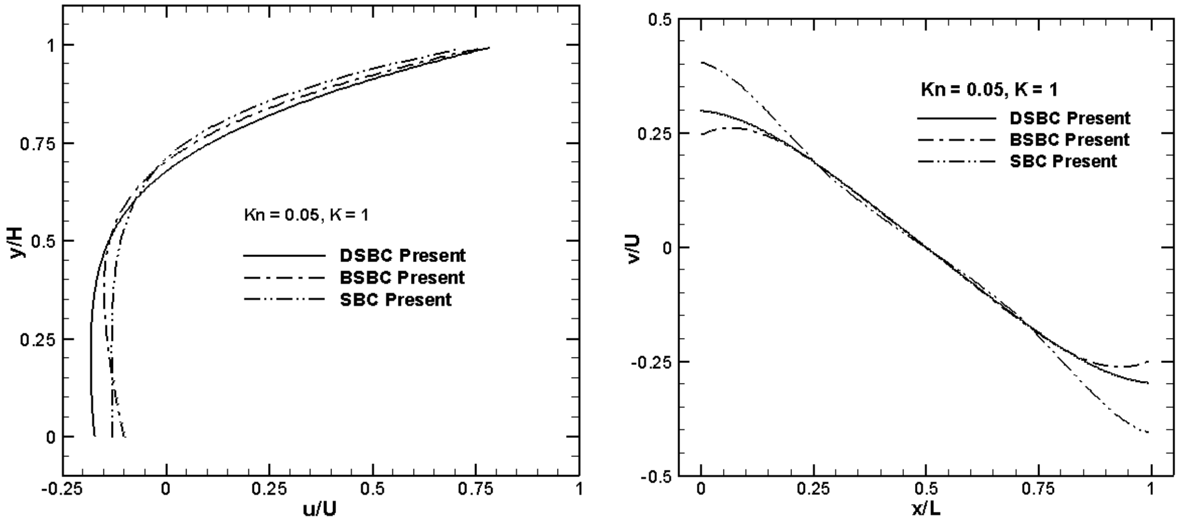


(a)



(b)

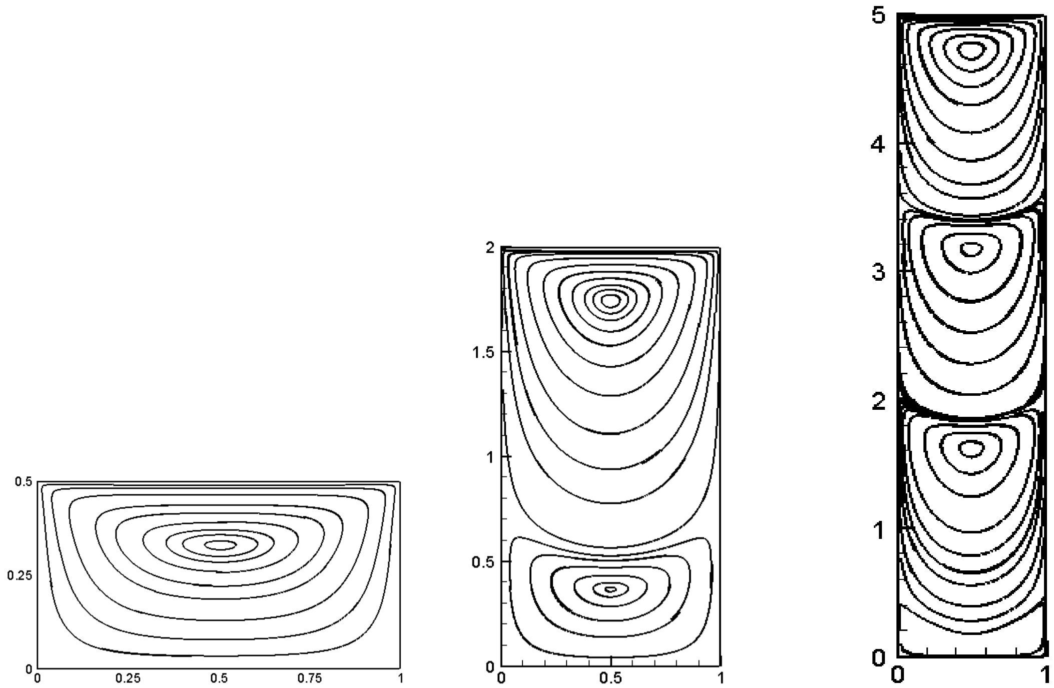
Figure 4. (a) *u*-velocity profile along the horizontal centreline and (b) *v*-velocity profile along the vertical centreline for different Knudsen numbers of the micro lid-driven square cavity flow. Lattice size: 300×300.



(a) (b)

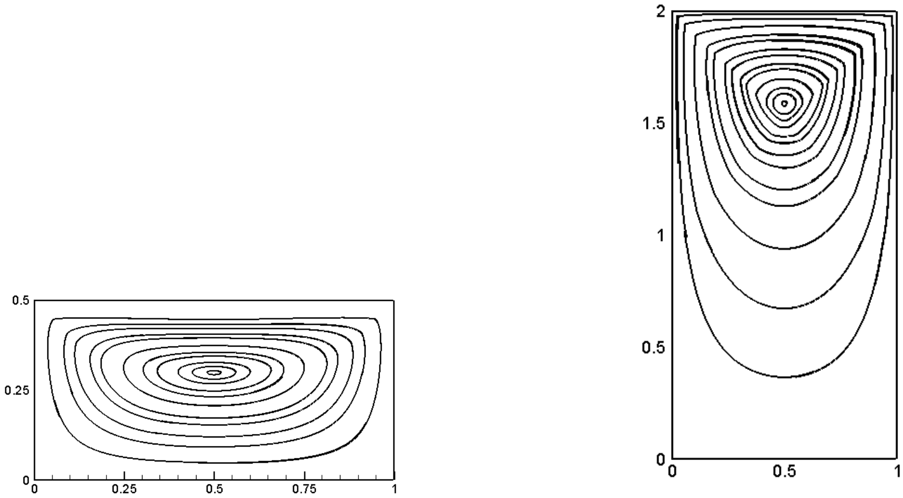
Figure 5. (a) u-velocity profile along the vertical centreline (b) v-velocity profile along the horizontal centreline for the micro-lid-driven square-cavity flow at Kn = 0.05 with the BSBC, SBC and DSBC boundary conditions. Lattice size: 300×300.

Figure 7 depicts the streamline patterns for micro lid-driven cavity flow at Kn = 0.10 (high-slip regime) with aspect ratios K = 0.5 and 2.0. Here it is seen that even at K = 2.0 there is only one vortex. Thus the present study reveals the fact that multiple vortices may be absent even at higher cavity-aspect ratios if the Knudsen number is relatively high. Another point is that a primary vortex appears in the cavity in all examined aspect ratios even at relatively large Knudsen numbers. This is along expected lines as at the lowest Knudsen number the ability of the top wall to drive the flow is at its highest and it generates the highest clockwise circulation. For all Knudsen numbers the present streamline patterns agree well with those reported by Darbandi *et al.* [13].



(a) K = 0.5 (b) K = 2.0 (c) K = 5.0

Figure 6: Streamline patterns for the micro-lid-driven cavity flow with aspect ratios K = 0.5, 2.0 and 5.0 at Kn = 0.01.



(a) $K = 0.5$ (b) $K = 2.0$

Figure 7: Streamline patterns for the micro-lid-driven cavity flow with aspect ratios $K = 0.5$ and 2.0 at $Kn = 0.10$.

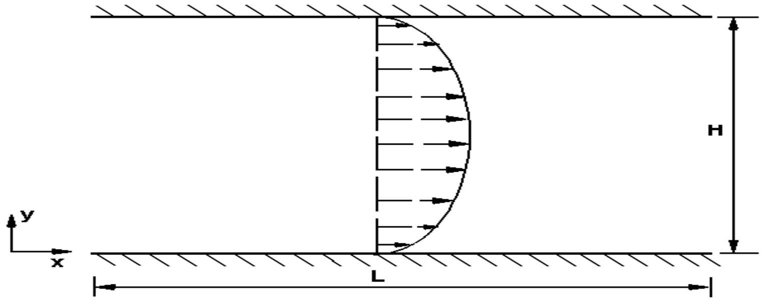


Figure 8. The geometry and micro-poiseuille flow profile.

3.3. Micro-poiseuille flow

Lattice Boltzmann Method is now used to investigate the isothermal micro-poiseuille flow. In this case, fully developed pressure driven flow between parallel plates is considered. The geometry and the micro-poiseuille flow profile is shown in Figure 8.

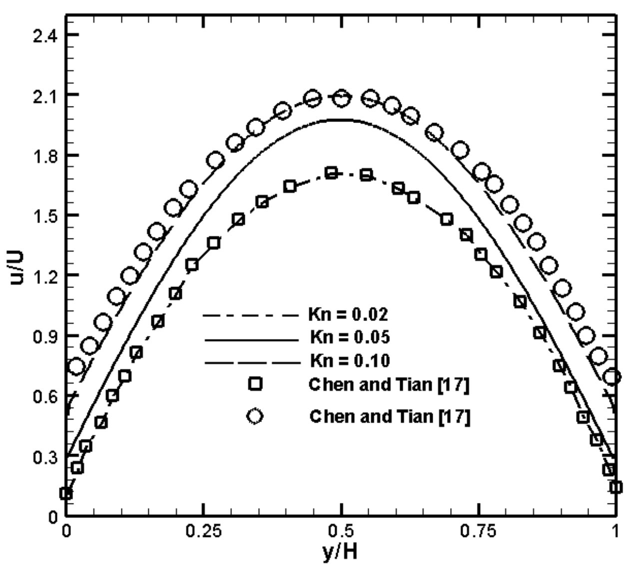


Figure 9. Velocity profiles of micro-poiseuille flow for various values of the Knudsen number.

Initially the *x*-direction velocity is assumed to be uniform through out the channel and *y*-velocity is taken as zero. Density is fixed at a value of 1.0 at inlet. Periodic boundary conditions are applied in the inlet and outlet. Combination of bounce-back and specular reflection (BSBC) boundary condition is used on the stationary walls. Figure 9 shows the velocity profiles of micro-poiseuille flow for different Knudsen numbers for a pressure ratio of 2.0 and $\sigma = 0.7$. For the sake of comparison, in the same figure we also plot the recently computed results of Chen and Tian [17], who used the lattice Boltzmann method with Langmuir slip model. The comparison exhibits good agreement. It is seen that, the highest value of horizontal velocity is in the middle of the channel and the horizontal velocity slows down near the two plates. As the Knudsen number increases, the slippage also increases. The effect of TMAC on the velocity profile at $Kn = 0.055$ is also studied and the results are depicted in Figure 10. As TMAC decreases, expectedly slip at the wall increases and the rate of increment in slip velocity is more as TMAC approaches zero.

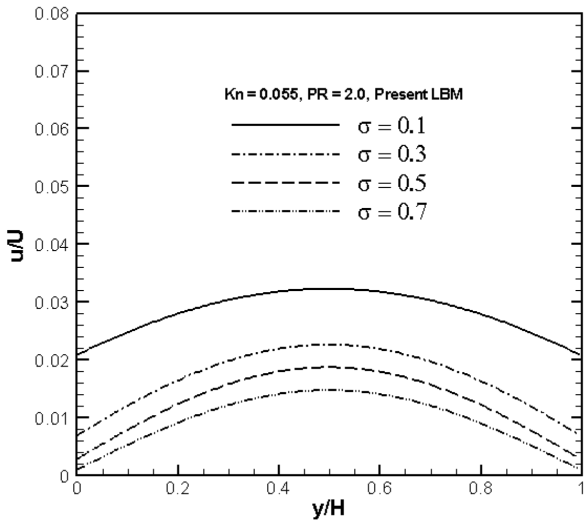


Figure 10. The effect of different TMAC on velocity profile of micro-poiseuille flow at $Kn = 0.055$.

4. Conclusion

The application of the LBM to compute rarefied gaseous flows in microgeometries is presented in this work. For the first geometry, namely, micro-couette flow some numerical and experimental results exist, which are reproduced with the LBM. This knowledge is then utilized when applying the LBM to compute flows in the second geometry, namely, a two-dimensional micro lid-driven cavity flow. Then the effect of Knudsen number with different boundary conditions is studied through the computation of flow in the micro lid-driven cavity. Results are presented for Knudsen numbers within the slip and the threshold of the transition regime where the onset of non-equilibrium effects are usually observed. Good agreement is found in predicting the general features of the velocity flow field and recirculating flow. Variation of slip with Knudsen number is then studied in some details through the computation of flow in the micro-poiseuille flow. To sum up, the present study reveals many interesting features of micro-couette, micro lid-driven cavity and micro-poiseuille flow and demonstrates the capability of the LBM to capture this features. It can be concluded that the present LBM, as an alternative to the particle based methods such as Molecular Dynamics and Direct Simulation Monte Corlo, holds very good promise in gaseous microflows.

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