

Simulation of Micro-Channel and Micro-Orifice Flow Using Lattice Boltzmann Method with Langmuir Slip Model

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ABSTRACT: Because of its kinetic nature and computational advantages, the Lattice Boltzmann method (LBM) has been well accepted as a useful tool to simulate micro-scale flows. The slip boundary model plays a crucial role in the accuracy of solutions for micro-channel flow simulations. The most used slip boundary condition is the Maxwell slip model. The results of Maxwell slip model are affected by the accommodation coefficient significantly, but there is not an explicitly relationship between properties at wall and accommodation coefficient. In the present work, Langmuir slip model is used beside LBM to simulate micro-channel and micro-orifice flows. Slip velocity and nonlinear pressure drop profiles are presented as two major effects in such flows. The results are in good agreement with existing results in the literature.

KEYWORDS: Lattice Boltzmann method; Langmuir slip model; Micro-channel; Micro-orifice

Introduction

Study on Micro-electro-mechanical-systems (MEMS) changed to an attractive research field in last two decays [1-2]. Application of such systems varies from automotive industry to aerospace, medical, military and telecommunications utilizations. Micro-channels, micro-pumps, micro-filters and micro-nozzles are some of commonly used micro-fluidic devices in MEMS. These systems usually involves gaseous flows and the behavior of these flows has significant effects on the performance of MEMS [3]. A dimensionless parameter, Knudsen number, categorizes flows with respect to that continuum assumption is applicable or not. The Knudsen number is ratio of the gas mean free path λ to the characteristic length of flow domain L ($Kn = \lambda/L$). The mean free path is the distance that a gas particle must travel between two consecutive collisions with other particles. If $Kn \leq 0.001$ the general Navier-Stokes equation can describe the flow and the non-slip boundary condition is applicable for boundaries (continuous regime). By reducing the size of flow domain, Kn increases and we will see some effects of rarefaction on the flow field. Most important effects are velocity slip and temperature jump on solid boundaries [4]. In the slip flow regime ($0.001 \leq Kn \leq 0.1$) the Navier-Stokes equation can be used to solve the domain, but the slip conditions must be accounted on the solid boundaries. In the transition ($0.1 \leq Kn \leq 10$) and free molecule ($Kn > 10$) regimes, the continuum assumption breaks down and some other methods such as Molecular Dynamics

(MD), Direct Simulation Monte Carlo (DSMC) must be used to solve the flow domain. Since the MD is limited in both length and time scales due to computational reasons, it is not a good choice for practical situations simulations.

In the recent years, the lattice Boltzmann method (LBM) has considered as an alternative strong tool for simulating micro scale flows [5]. The computational cost of LBM is comparable to that of Navier-Stokes solvers [6]. So it is faster than MD and DSMC [7]. Moreover LBM can be applied in wider region proportional to Navier-Stokes solvers theoretically [8]. Implementation of slip boundary condition is one of the most important aspects of using LBM for micro flows. Different boundary condition treatments have been reported [9], but the most used slip boundary model is the Maxwell slip model. Velocity slip determination in this model is by the accommodation coefficient, Knudsen number and the gradient of the velocity [10]. The results of Maxwell slip model are affected by the accommodation coefficient significantly, but there is not an explicitly relationship between properties at wall and accommodation coefficient. Results of other models, experimental results for example, must be used for setting this coefficient. Moreover the slip velocity can become unbounded [11]. One alternative boundary condition treatment is Langmuir slip model. In this model gas molecules do not reflect directly, but will be remained on the surface for a brief period of time [12]. Langmuir model recovers the Maxwell model in its first-order approximation [13] and therefore the accommodation coefficient can be described physically. Some researchers have used LBM in their simulations of gaseous micro flows.

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Nomenclature			
f	distribution function	η	relaxation time
t	time	α	constant of model
c	vector of particle velocity	β	reaction constant
e	discrete velocity	ω	constant of model
u	macroscopic velocity		Superscripts
x	horizontal space coordinate of lattice	eq	equilibrium
w	equilibrium distribution weight	\sim	model parameter
N	number of lattice nodes	+	model parameter
Kn	Knudsen number	slip	Slip
p	pressure	neq	non-equilibrium
y	vertical space coordinate of lattice		Subscripts
L	length	i	lattice direction
PR	pressure ratio	g	adjacent to wall
	Greek Symbols	w	wall
τ	relaxation time	o	outlet
Ω	collision operator	f	momentum
ρ	density	*	normalized

Nie et al. [14] simulated two-dimensional micro channel and micro driven cavity flows using LBM with bounce-back boundary condition in the no-slip and slip regimes. Tang et al [15] applied a boundary condition based on the kinetic theory to simulate gaseous slip flow in micro geometries. Zhang et al. [16] used the accommodation coefficient to describe gas-surface interactions. Shirani and Jafari [17] used a combination of bounce-back and specular boundary conditions. Myong et al. [18] studied micro scale cylindrical couette flow using Langmuir slip model and showed that this model is in qualitative agreement with DSMC method. Kim et al. [10] showed how to implement the Langmuir slip model by bounce back scheme. Chen and Tian [19] proposed a boundary condition based on the Langmuir slip model to simulate micro channel and micro couette flows. Chen and Tian [20] also investigated thermal micro flow using Langmuir slip model. They showed how to implement the Langmuir slip model for the LBM to capture velocity slip and temperature jump in micro flows with temperature difference. Despite it's better physically explanations, surprisingly there are a few attempts to implement Langmuir slip model to complicated geometries like micro-orifices. The aim of this study is to show velocity increasing at the orifice and velocity slip on the walls for the flow passing through a micro orifice. But first the results are gained for micro-channel flow and credibility of LBM code is tested for a flow in a long micro-channel.

Numerical Model

The Lattice Boltzmann Method

LBM can be presented as a discrete version of the Boltzmann theory. Time, space and momentum all are discretized in this particular scheme of Boltzmann equation, equation 1.

$$\frac{\partial f}{\partial t} + c \cdot \nabla f = -\frac{1}{\tau} (f - f^{eq}) \quad (1)$$

C is the vector of particle velocity. f^{eq} is the equilibrium distribution function and τ is the relaxation time. In LBM particles are modeled by distribution functions and these particles can move only in certain and fixed directions in a lattice domain. In this work the velocity space discretization is the D2Q9 model which is the most popular model for the 2D case [21].

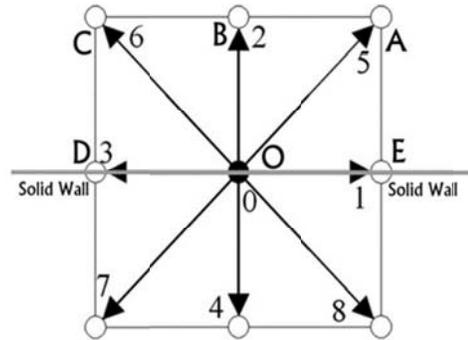


Fig. 1. D2Q9 model at a wall boundary

The particles can move along the eight moving directions to neighboring lattice cells or can be in a stationary state in the center of lattice cell. Figure 1 shows the 9 velocities of the D2Q9 model. This model to simulate the dynamics of fluid particles can be represented by the Lattice Boltzmann Equation (LBE), equation 2.

$$f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = \Omega_i(f) \quad (2)$$

Here, Ω_i is the collision operator. This operator in the Bhathagar-Groos-Krook (BGK) model with single relaxation time simplifies and the BGK Lattice equation can then be presented as:

$$f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau} [f_i(x, t) - f_i^{eq}(x, t)] \quad (3)$$

e_i are the discrete velocity set:

$$e_i = (0,0), i = 0$$

$$e_i = c(\cos[(i-1)\pi/4], \sin[(i-1)\pi/4]), i = 1,2,3,4 \quad (4)$$

$$e_i = \sqrt{2}c(\cos[(i-1)\pi/4], \sin[(i-1)\pi/4]), i = 5,6,7,8$$

Here, $c = \Delta x / \Delta t$ is the particle streaming velocity. Δx and Δt are constant lattice space and the time steps respectively. The equilibrium distribution function for the D2Q9 model is expressed as [25]:

$$f_i^{eq} = w_i \left(1 + \frac{3}{c^2} e_i \cdot u + \frac{9}{2c^4} (e_i \cdot u)^2 - \frac{3}{2c^2} u \cdot u \right) \quad (5)$$

Where w_i is the equilibrium distribution weight for direction i and equals to 4/9 for $i = 0$ and 1/9 for $i = 1,2,3,4$ and 1/36 for $i = 5,6,7,8$.

The fluid density, ρ , can be evaluated with equation 6, whereas the velocity, u , is contained in the momentum fluxes of equation 7:

$$\rho = \sum_i f_i \quad (6)$$

$$\rho u = \sum_i e_i f_i \quad (7)$$

Equation 3 is usually solved in two steps, based on the work of Chen and Tian [20] these two steps can be presented as:

$$\text{Collision: } \tilde{f}_i^+(x, t) = (1 - \eta_f) \tilde{f}_i(x, t) + \eta_f f_i^{eq}(x, t) \quad (8)$$

$$\text{Streaming: } \tilde{f}_i(x + e_i \Delta t, t + \Delta t) = \tilde{f}_i^+(x, t) \quad (9)$$

where $\eta_f = \Delta t / (\tau_f + 0.5\Delta t)$ and τ_f is the momentum relaxation time. The new variable \tilde{f}_i is defined as $\tilde{f}_i = f_i + (0.5\Delta t (f_i - f_i^{eq}) / \tau_f)$.

The first step is called collision. In this step fluid particles interactions are modeled and new distribution functions according to the distribution functions of the last time step and the equilibrium distribution functions will be calculated with equation 5. The second step is called streaming step. Fluid particles are streamed from one cell to a neighboring cell according to the velocity of the fluid

particles in this step. To implement Lattice Boltzmann method for micro flows we first need to define a relationship between Knudsen number Kn and the relaxation time, τ . Various relationships have been proposed. A simplified relation for the standard D2Q9 lattice BGK model is presented at [22]:

$$Kn = \frac{\sqrt{\pi}}{\sqrt{6}} \cdot \frac{(\tau - 0.5)}{N_y \Delta t} \quad (10)$$

Langmuir Slip Model

In the Langmuir slip model interactions between gas molecules and solid wall atoms are accounted in boundaries. There are intermolecular forces between the gas molecules and the solid surface atoms. So the gas molecules don't reflect directly into the flow but reside for a brief period of time at wall.

In fact these molecules can be adsorbed onto the surface, and then desorbed after some time lag. This time lag leads to macroscopic velocity slip. In the Langmuir slip model the velocity slip can be expressed as [23]:

$$\vec{u}^{slip} = (1 - \alpha) \vec{u}|_g + \alpha \vec{u}|_w \quad (11)$$

Where $\vec{u}|_w$ and \vec{u}^{slip} are the velocity of the wall and gas velocity at the wall respectively and subscript g represents being adjacent to the wall.

The coefficient α varies with the type of the gas and the nature of the wall material.

$$\alpha = \frac{\beta p}{1 + \beta p} \quad (12)$$

for monatomic gases and

$$\alpha = \frac{\sqrt{\beta p}}{1 + \sqrt{\beta p}} \quad (13)$$

for diatomic gases. β is the reaction constant for surface-gas molecules and is defined as

$$\beta = 1/4\omega Kn \quad (14)$$

ω has a role very similar to the accommodation coefficient in the Maxwell slip model, but we can determine its value with a clear physical explanation [19] and p is the pressure. By combining equations 12 and 14:

$$\alpha = \frac{1}{1 + 4\omega Kn/p} \quad (15)$$

Implementation of Langmuir slip model for the LBM model

In general, the distribution function can be decomposed into equilibrium and non-equilibrium parts:

$$\tilde{f}_i(x, t) = f_i^{eq}(x, t) + f_i^{neq}(x, t) \quad (16)$$

For south boundary nodes, the density distribution functions in e_2 , e_5 and e_6 directions are unknown before streaming step (Figure 1).

Treatment for Langmuir slip model at the boundary node O on the south wall and e_2 direction will be present [20]. The post-collision density distribution function can be assumed as

$$\tilde{f}_2^+(O, t) = F_2^{eq}(O, t) + (1 - \eta_f)F_2^{neq}(O, t) \quad (17)$$

Using Langmuir slip model, the natural choice for $F_2^{eq}(O, t)$ is

$$F_2^{eq}(O, t) = \alpha f_2^{eq}(W, t) + (1 - \alpha)f_2^{eq}(B, t) \quad (18)$$

And

$$F_2^{neq}(O, t) = \alpha f_2^{neq}(W, t) + (1 - \alpha)f_2^{neq}(B, t) \quad (19)$$

$f_2^{eq}(W, t)$ can be approximated as

$$f_2^{eq}(W, t) = f_2^{eq}(\rho(B), u(w), t) + \mathcal{O}(\varepsilon^2) \quad (20)$$

Where ε is a slight quantity.

Equations for calculating non-equilibrium parts are given by

$$f_2^{neq}(B, t) = f_2(B, t) - f_2^{eq}(B, t) \quad (21)$$

And

$$f_2^{neq}(W, t) = f_2(B, t) - f_2^{eq}(B, t) + \mathcal{O}(\varepsilon^2) \quad (22)$$

Thus the final form of equation 17 becomes

$$\tilde{f}_2^+(O, t) = \alpha f_2^{eq}(\rho(B), u(W), t) + (1 - \alpha)f_2^{eq}(B, t) + (1 - \eta_f)[f_2(B, t) - f_2^{eq}(B, t)] + \mathcal{O}(\varepsilon^2) \quad (23)$$

Extension the method to other directions is straight forward.

Numerical results

Micro-Channel

As mentioned in Beskok et al. [24] there are two major effects, rarefaction and compressibility, occurred in micro scales for an isothermal flow. BGK Lattice Boltzmann method with D2Q9 model is used to simulate the micro-channel flow. Then the effects of rarefaction and compressibility can be shown by velocity and pressure profiles. The flow is driven by the pressure difference

imposed at inlet and outlet sections. So the pressure values at inlet and outlet are fixed with a specified pressure ratio ($PR = P_{inlet}/P_{outlet}$). The relationship between Kn and relaxation time is given in equation 24 and the local Kn can be evaluated by:

$$Kn(x)P(x) = Kn_o P_o \quad (24)$$

Here, Kn_o and P_o are the Kn number and pressure at outlet section respectively. All simulations for studying micro-channel flow are done on a 2100×21 domain which has been shown to be able to give mesh-independent results.

The compressibility effect in micro channel can be performed by pressure distribution along the flow direction. Figure 2 shows nonlinearity of pressure along the channel. In this figure P/P_o is plotted against x/L for $PR=1.94$ and various Kn numbers. For a specified Kn, the pressure decreases in the streamwise direction in a micro-channel.

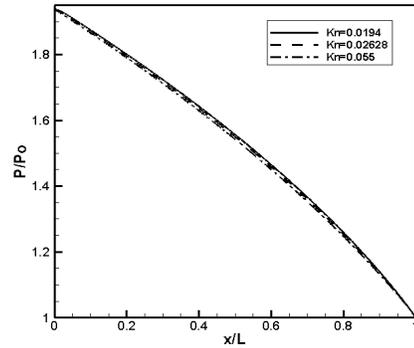


Fig. 2. Non-dimensionalized pressure distribution at the center of the flow along the x direction

The deviation of normalized pressure from linear behavior, $(P-P_1)/P_o$, as a function of x/L is shown in the figure 3, where $P_1 = P_o + (P-P_o)(1-x/L)$. The results of present work agree well with results of Karandakis [2] for $Kn = 0.0194$.

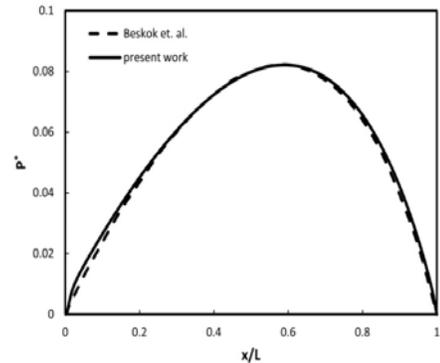


Fig. 3. Non-linearity of the pressure distribution along the micro-channel

Deviations of the pressure distribution for the same Kn_0 and different inlet pressures are plotted in figure 4. By increasing the inlet pressure, the compressibility within the channel increases and the deviation from linear distribution must become larger.

This fact is clearly observable in figure 4. Another point that we can understand from this plot is moving the location of maximum deviation toward the channel exit by increasing the inlet pressure.

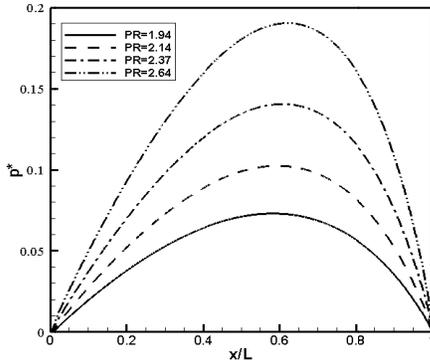


Fig. 4. Nonlinearity of pressure along the channel for $Kn_0=0.055$ and different inlet pressures

Figure 5 shows the effect of various Kn_0 on the pressure deviation from linear distribution. As indicated in the figure, the larger value for Kn_0 leads to a smaller deviation in the pressure distribution.

So the rarefaction effects want to decrease the curvature of the pressure distribution that is a result of the compressibility effect. This means that the pressure distribution along the channel is somewhat balance between compressibility effect and rarefaction effect.

Equation 24 shows the relation between the local pressure and the local Knudsen number.

With the decreasing pressure along the flow direction, the local Knudsen number must be increased. The local Knudsen numbers along the flow direction are plotted in the figure 6.

The maximum value of Knudsen number occurs at the outlet section of the micro-channel.

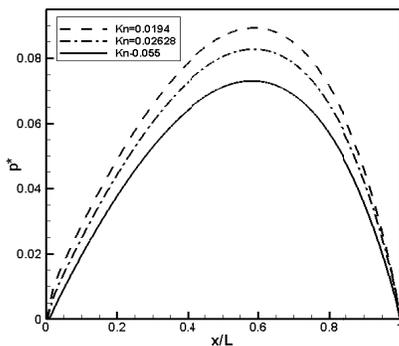


Fig. 5. Nonlinearity of pressure along the channel for different Knudsen numbers

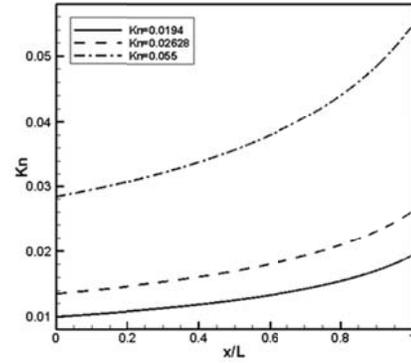


Fig. 6. The local Knudsen numbers along the flow direction

The effect of various inlet pressures on the distribution of local Knudsen numbers is shown in figure 7. With increasing the inlet pressure, decreasing the local Knudsen numbers in the inlet and other sections across the channel is observed.

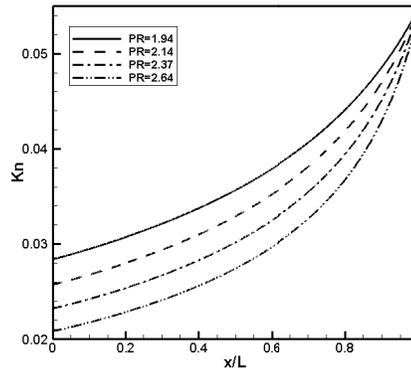


Fig. 7. The effect of various inlet pressures on the local Knudsen numbers along the flow direction for $Kn_0=0.055$

Figure 8 represents the normalized streamwise velocity, u/U , where U is the average velocity for $Kn_0=0.0194$ and $PR=1.94$. Comparing the results of present work with those of Reis and Dellar [26] for same values of Kn_0 and PR shows reasonably good agreement between them. There is a slip velocity at both upper and down boundary walls in the figure.

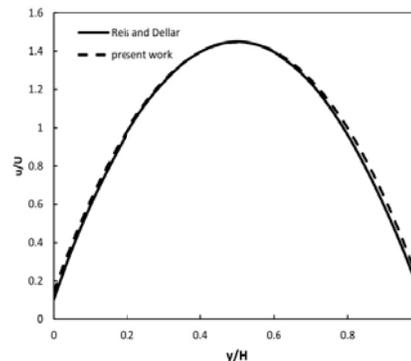


Fig. 8. Normalized streamwise velocity for $Kn_0=0.0194$

Vectors of streamwise velocities in the micro-channel are plotted in figure 9 for $Kn_o=0.0194$ and $PR=1.94$.

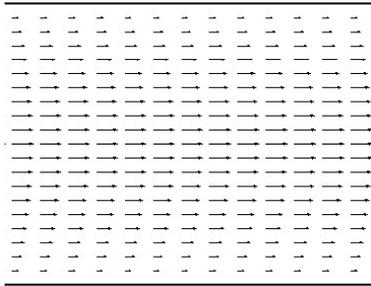


Fig. 9. The vectors of streamwise velocities in micro-channel for $Kn_o=0.0194$ and $PR=1.94$

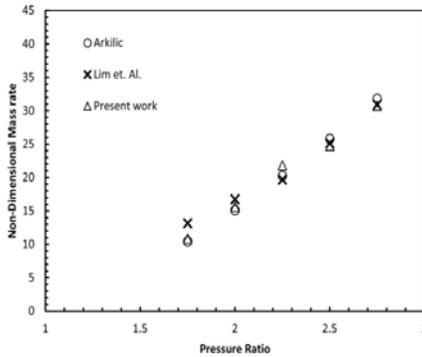


Fig. 10. The non-dimensionalized mass flow rate per unit width of micro-channel for $Kn_o=0.05$

Micro-orifice

BGK Lattice Boltzmann method with D2Q9 then used to simulate flow passing through a micro-orifice. The ratio of the open orifice area to the total area is 0.6. The geometry of micro-orifice is showed in the figure 11.

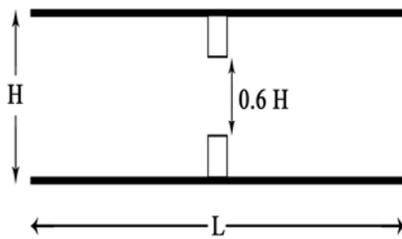


Fig. 11. The geometry of micro-orifice

In Figure 12, the computed u-velocity profile at orifice is compared with the results of Wang and Li [27] for $PR=1.5$. The results of the present work agree quantitatively well with their numerical results.

The simulations are performed at atmospheric conditions, with air assumed to flow through the micro orifice. Simulations have isothermal conditions where the temperature of the micro orifice and surrounding areas is kept at 298 K. The pressure at inlet and outlet sections of channel set to be constant and the flow is driven by the

difference between them. Langmuir slip model is implemented on channel and orifice walls.

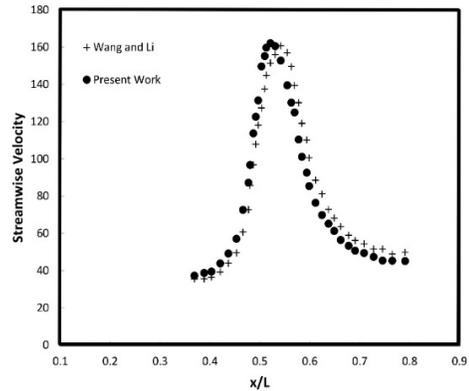


Fig. 12. Streamwise velocity at Orifice for $PR=1.5$

The length and height of the channel are 2000 and 21 lattice nodes respectively and the orifice is located symmetrically in the channel.

Figure 13 shows the streamwise velocity distribution against streamwise direction, x . When the flow approaches the orifice accelerates and the maximum value of streamwise velocity take occurs at the orifice section. Increasing the Knudsen number results to a decrease in streamwise velocity along the channel. It seems that the rarefaction effects tend to decrease the maximum value of the streamwise velocity at the orifice.

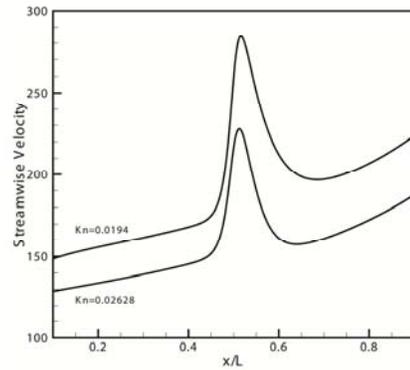


Fig. 13. Streamwise velocity for two different Knudsen numbers

The effect of different inlet pressures on streamwise velocity is represented in figure 14.

As showed before, the velocity increases along flow direction through the channel and reaches to its maximum value at the outlet section of the channel. So if we locate the orifice in various locations, the maximum value of streamwise velocity must change. This fact is represented by figure 15. The orifice is located at three different locations ($x/L=0.25$, $x/L=0.5$ and $x/L=0.75$) and the highest value of streamwise velocity increases as the orifice is shifted into the outlet of the channel.

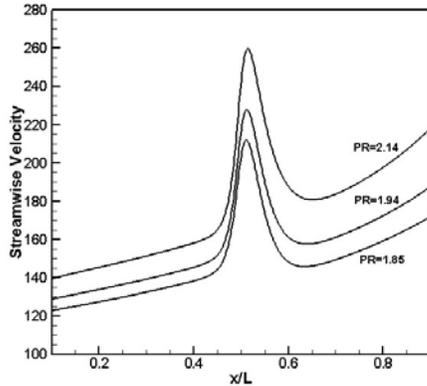


Fig. 14. Streamwise velocity for $Kn_0=0.02628$ and different inlet pressures

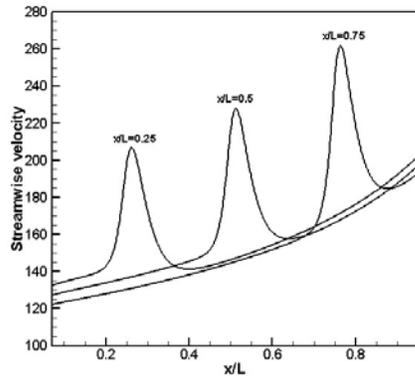


Fig. 15. Streamwise velocity for $Kn_0=0.02628$ and different locations of orifice

At last streamlines at the orifice section are plotted in the figure 16.

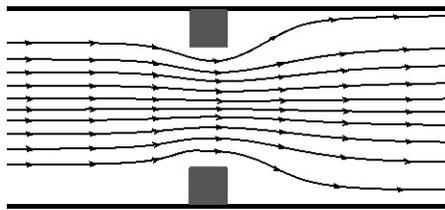


Fig. 16. Streamlines at orifice section for $Kn_0=0.0194$ and $PR=1.94$

Conclusions

Langmuir slip model is an alternative boundary condition with better physical explanations beside commonly used Maxwell slip model. But surprisingly is not used to simulate complicated geometries like micro-orifice flows. The main aim of this work is to show the ability of Longmuir slip model to predict the flow behaviour in complex micro-flows. Lattice Boltzmann method is used to simulate isothermal two dimensional micro-channel and micro-orifice flows. The Langmuir slip model is implemented to solid boundaries of mentioned geometries and the flow is driven by the difference of constant pressures at inlet and outlet sections of channel. To

showing the effects of rarefaction and compressibility, velocity and pressure profiles are plotted for various situations. Slip velocity and non-linearity of pressure distribution are gained successfully in our simulations. Some results of present work are compared with those exists in the literature and they enjoy good credibility.

In the case of micro-orifice flow, the suddenly increase of streamwise velocity in the contraction region and the effects of various Knudsen numbers, different inlet pressures and locations of orifice are shown in the profiles of streamwise velocity along the flow direction.

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