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Simulation of Rarefied Gas Flow in Slip and Transitional Regimes by the Lattice Boltzmann Method

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Abstract

In this paper, a lattice Boltzmann method (LBM) based simulation of microscale flow has been carried out, for various values of Knudsen number. The details in determining the parameters critical for LBM applications in microscale flow are provided. Pressure distributions in the slip flow regime are compared to the analytical solution based on the Navier-Stokes equation with slip-velocity boundary condition. Satisfactory agreements have been achieved. Simulations are then extended to transition regime (Kn = 0.15) and compared with the same analytical solution. The results show some deviation from the analytical solution due to the breakdown of continuum assumption. From this study, it can be concluded that the lattice Boltzmann method is an efficient approach for simulation of microscale flow.

Keywords: Distribution function; Boltzmann equation; BGK collision model; microscale flow; microchannel

1. Introduction

In recent years, many of the researchers have diverted their attention to the microscale flow area [1-4]. Microscale flows are defined as fluid flow phenomena associated with microscale mechanical devices. While understanding these phenomena is of great fundamental interest, there are also major economical incentives related to many industrial applications such as micro-electro mechanical system (MEMS), micro heat exchanger, micro pump, etc. Flow in micro devices with characteristic size of the order of microns differ from their large counterparts. Two important flow parameters; Knudsen number Kn, and Reynolds number Re, are drastically different from those encountered in large scale flows [5-7]. Experimental work on such microscale behavior is very difficult and expensive if not impossible because of the length- and time-scale involved. Due to these reasons, it is necessary to establish a numerical model which can exactly simulate the flow characteristics at microscale condition. Currently, the lattice Boltzmann method is the most suitable numerical tool in simulating microscale

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fluid flow problem.

The lattice Boltzmann method (LBM), the numerical method that will be used in this study, is the only numerical technique that directly treats the flow behaviour at microscopic level. LBM utilizes the particle distribution function to describe collective behavior of fluid molecules. This new numerical method, evolved from mathematical statistical approach, has been well accepted as an alternative numerical scheme in computational fluid dynamics field. In comparison with other numerical schemes, LBM is a "bottom up" approach, derives the Navier-Stokes equation from statistical behavior of particles dynamics. The imaginary "propagation" and "collision" processes of fluid particles are reconstructed in the formulation of LBM scheme. These processes are represented by the evolution of particle distribution function $f(x,t)$, which describes the statistical population of particles at location x and time t.

The advantages of LBM include simple calculation procedure [8], suitability for parallel computation [9], ease and robust handling of multiphase flow [10], complex geometries [11], interfacial dynamics and others [12-13]. A few standard benchmark problems have been simulated by LBM and the results are found to agree well with the corresponding Navier-Stokes solutions [14-16].

The attractiveness of LBM in simulating microscale flow lies in the fact that, unlike other conventional scheme, no special treatment or attention is required for the solid boundaries, meaning that no extra computational burdens is needed to apply slip boundary condition at solid boundaries [17]. Thus, the LBM is an ideal tool in predicting microscale flow phenomena. Application of LBM is expected to increase the efficiency, accuracy and the capability of the current computer performance without scarificing the need of the detailed behavior of fluid particles for this type of flow.

There were works have been carried out to understand microscale flow behavior experimentally and numerically. In 1997, Arkilic et al [4] investigated the gaseous flow through long microchannel. They found that the rarefaction and compressibility effect can be reproduced by applying first order slip boundary condition in the solution to two-dimensional Navier-Stokes equation.

In order to gain better understanding on the behavior of fluid flow at particle level, Xue et al, [18] used Direct Simulation Monte Carlo method (DSMC) to predict microchannel flow. They claimed that the DSMC can go beyond the capability of Navier-Stokes method to simulate at high Knudsen number when the continuum assumption is no longer valid. However, DSMC is reported to consume very long computational time even to predict the evolution of particle in a small physical geometry [19].

The application of LBM in predicting microscale flow is relatively new. Xiaobo et al, [20] firstly introduced LBM to simulate flow in MEMS. Zhang et al, [5] and Lim et al, [21] applied slip boundary condition to describe gas-surface interaction in microchannel by introducing tangential momentum accommodation coefficient. Their results are compared well with the analytical solution provided by Arkilic et al, [4]. However, the simplicity property of the lattice Boltzmann scheme has been lost due to this complicated boundary treatment.

In the work reported by Frederik et al, [22], who investigated the flow behavior in long microchannel using LBM, they demonstrated that the conventional bounce-back boundary condition [23] still valid for no-slip boundary condition at the walls. Their results compared well with the analytical solution of Navier-Stokes equation and DSMC method. Recently, Agrawal et al [17] proved the capability of bounce-back boundary condition of LBM to simulate flow in microchannel for simple and complex boundaries.

This paper is differentiated from previous microchannel studies by inclusion of density dependence relaxation time in LBM formulation to reproduce compressibility and rarefied effects. In order to maintain the simplicity of LBM, we applied the original bounce-back boundary condition for the wall boundary treatment. Other than that of two-dimensional isothermal fluid flow, no assumptions regarding the flow profile or distribution of pressure are made. The results of pressure distribution along the channel are then plotted and compared with the analytical solution.

The rest of the paper is organized as follow. Section 1 discusses the formulation of lattice Boltzmann method. After showing how the formulation of LBM fits in to the framework of microscale

flow, numerical results of microchannel flow at various Knudsen number are presented to highlight the applicability of the approach. The final section concludes current study.

2. Isothermal Lattice Boltzmann Model

Historically, LBM is the logical development of lattice gas automata (LGA) method [24]. Like in LGA, the physical space is discretized into uniform lattice nodes. Every node in the network is then connected with its neighbours through a number of lattice velocities to be determined through the model chosen.

The lattice Boltzmann equation is given by:

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

where $f = f(x,t)$ is the distribution function for particles with velocity e at position x and time t.

Equation (1) consists of two parts: propagation (left hand side) which refers to the propagation of distribution function to the next node in the direction of its probable velocity, and collision (right hand side) which represents the collision of the particle distribution function. In LBM, magnitude of e is set up so that in each time step Δt, every distribution function propagates in a distance of lattice nodes spacing Δx. This will ensure that distribution function arrives exactly at the lattice nodes after Δt and collide simultaneously. Note that Bhatnagar-Gross-Krook (BGK) collision model [25] with single relaxation time is used for the collision term where f^{eq} is the equilibrium distribution function and t is the time to reach equilibrium condition during collision process.

The general form of the lattice velocity model is expressed as *DnQm* where *D* represents spatial dimension and *Q* is the number of connection (lattice velocity) at every node. In this paper, the nine-microscopic velocity or nine-bit model (*D2Q9*) is used. The discrete velocity is expressed as:

$$\begin{aligned} e_0 &= (0,0) \\ e_{1,3,5,7} &= \left(cos\frac{(i-1)\pi}{4}, sin\frac{(i-1)\pi}{4}\right) \\ e_{2,4,6,8} &= \sqrt{2}\left(sin\frac{(i-1)\pi}{4}, cos\frac{(i-1)\pi}{4}\right) \end{aligned} \tag{2}$$

The equilibrium distribution function of the nine-bit model is [26]:

$$f^{eq}=\rho\omega_i\left[1+3c_i\cdot u+\frac{9}{2}\left(c_i\cdot u\right)^2-\frac{3}{2}u^2\right] \tag{3}$$

where the weights are:

$$\omega_0=\frac{4}{9},\omega_{1,3,5,7}=\frac{1}{9},\omega_{2,4,6,8}=\frac{1}{36} \tag{4}$$

The macroscopic variables, such as density , and velocity u can be evaluated as the moment to the distribution function as follow:

$$\rho=\Sigma_i f_i \tag{5}$$

$$u=\frac{\Sigma_i c_i f}{\Sigma_i f_i} \tag{6}$$

$$P=\frac{1}{3}\rho \tag{7}$$

The viscosity is related to the relaxation time through:

$$\upsilon=\frac{2\tau-1}{6} \tag{8}$$

In microscale flows, the local density variation is relatively small, however the total density changes, for instance the density difference between the inlet and outlet of a very long channel could be quite large. To include the dependence of viscosity on density, we replace τ by τ' as follow:

$$\tau' = \frac{1}{2} + \frac{1}{\rho}\left(\tau - \frac{1}{2}\right) \tag{9}$$

From above explanation, we can see that the LBM is a suitable choice for simulation of microscale flow. According to Shen et al, [27], LBM can be used at least up to $Kn \approx 0.2$. Even if we apply slip boundary condition, solution to Navier-Stokes equation only hold in the slip flow regime ($0.001 < Kn < 0.1$). Therefore LBM is better suited for microscale gas flow as compared to the conventional Navier-Stokes solver.

3. Microchannel Flow Simulation

In this section, we will discuss how to apply the lattice Boltzmann method to simulate microchannel flow. The computational domain employed in this study consists of two-dimensional channel with the channel width is resolved by 21 grid points. The aspect ratio is set up very high so that the density gradient between the successive grids is not very steep. This is to ensure the applicability of LBM is simulating hydrodynamics [28]. Note that we have not tried to provide physical dimension of the channel because the same results apply under identical values of the non-dimensional governing parameters.

The dynamical similarity depends on two non-dimensional parameters: The Knudsen number Kn, and Reynolds number *Re*. The Knudsen number, $Kn = l/H$, can be used to identify the influence of the effect of the mean free path on the flow, where l is the mean free path of the molecules and H is a typical dimension of the flow domain. As we have pointed out that for a system with $Kn < 0.001$, the fluid flow can be treated as continuum and can be easily solved by Navier-Stokes solution. As *Kn* increases, the flow enters the "slip-flow" ($0.001 < Kn < 0.1$) and "transition" ($0.1 < Kn < 3$) regimes. In the transition regime, the conventional flow solver, which is based on the computation of Navier-Stokes equations, is no longer applicable. The second non-dimensional parameter is the well-known Reynolds number, defined as:

$$Re = UH/\upsilon \tag{10}$$

Other than these two non-dimensional parameters, we need to carefully restrict LBM simulation parameters so that the low-Mach-number approximation holds. To do this, the third non-dimensional parameter, the Mach number *Ma*, is introduce and defined as U/c_s. In present scheme, the Knudsen, Reynolds and Mach numbers are related as follow:

$$Kn = 1.2533 Ma / \mathrm{Re} \tag{11}$$

Note that these numbers are computed during the post-processing of the data rather than being specified before start of the simulations. By combining (8), (10) and (11), the Knudsen number can be related to the relaxation time in LBM formulation as follow:

$$Kn = 0.0362\tau - 0.0181 \tag{12}$$

A conventional bounce-back boundary condition [23] is used at the top and bottom walls. According to this condition, the particle distribution function is considered fully rebound to its original position when it hits the wall after one iteration time step. For example:

$$f_3(x,1,t) = f_7(x,1,t-1) \text{ at lower wall} \tag{13}$$

$$f_7(x,H,t) = f_3(x,H,t-1) \text{ at upper wall} \tag{14}$$

Even with this simple boundary treatment, the bounce-back boundary condition allows slip at the wall for high Knudsen number [29].

The flow in microchannel is driven by the pressure gradient between the inlet and outlet of the channel. Pressure at the left is kept higher than the pressure at the right to induce a flow to the right. The pressure ratio has been fixed to two for the computations presented in this paper. By setting up

the value of pressure at the inlet (or outlet), the incoming distribution function can be calculated using the Dirichlet types boundary condition proposed by Zou and He [30].

4. Results and Discussion

Arkilic et al, [4] obtained analytical Navier-Stokes solution at low Kn with a first order slip model for two dimensional microchannel flow, in which the general pressure profile was describe. As predicted by Arkilic et al, [4], the pressure profile along the length of microchannel is expressed as a function of location in the microchannel direction and overall pressure ratio is:

$$P^* = -6\sigma Kn + \sqrt{(-6\sigma Kn)^2 + (1+12\sigma Kn)X + (\mathrm{Pr}^2 + 12\sigma Kn\,\mathrm{Pr})(1-x)} \qquad (15)$$

In the present study, four cases were simulated at different Knudsen number, *Kn = 0.02, 0.05, 0.1* and *0.15*. Once *Kn* is decided, the relaxation time can be calculated from (12). In each simulation, the output results are plotted when the difference of the value of centerline velocity at the outlet less than 10^{-5} for two successive iterations.

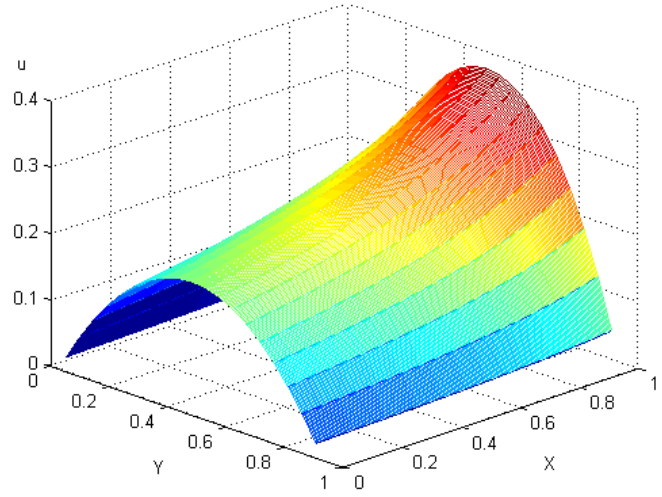


Figure 1. horizontal velocity profile for *Kn* = 0.05

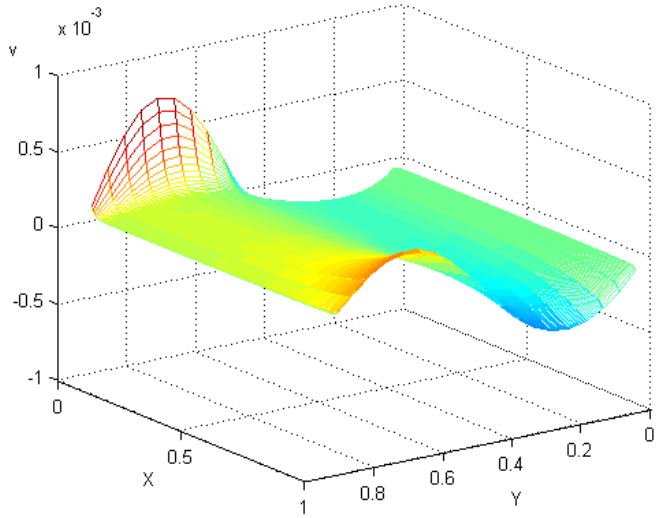
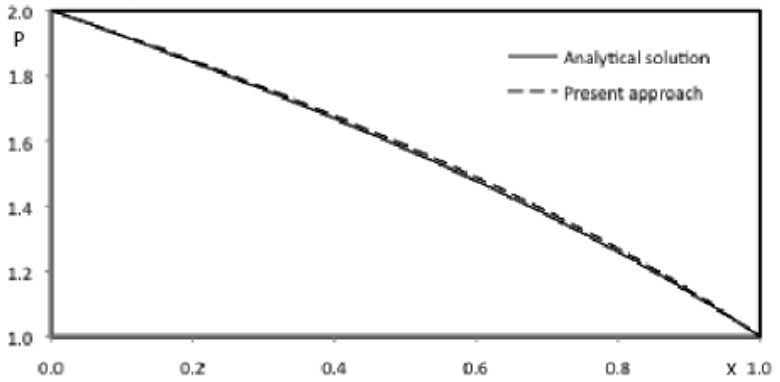


Figure 2. Vertical velocity profile for *Kn* = 0.05

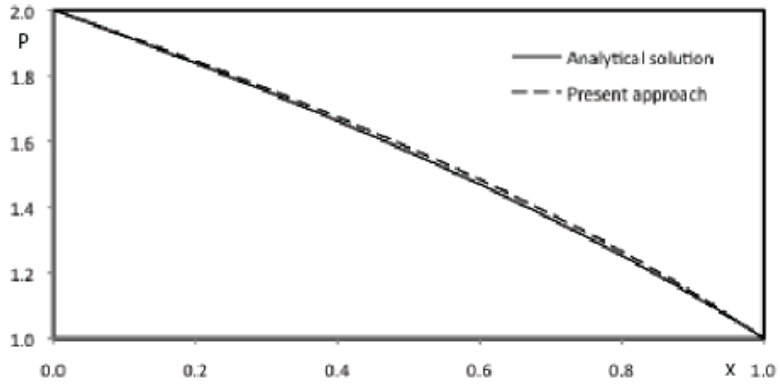
Figures 1 and 2 show the velocity profiles obtained by the proposed LBM formulation at Kn = 0.05. As can be seen for these figures, the horizontal velocity increases along the channel due to the pressure drop. However, vertical velocity along the channel is symmetric at the center. The magnitude of vertical velocity is very small and gives less significant to the flow characteristic in

the microchanel. All of these profiles show the similarity with the profiles published by Arkilic et al [4].

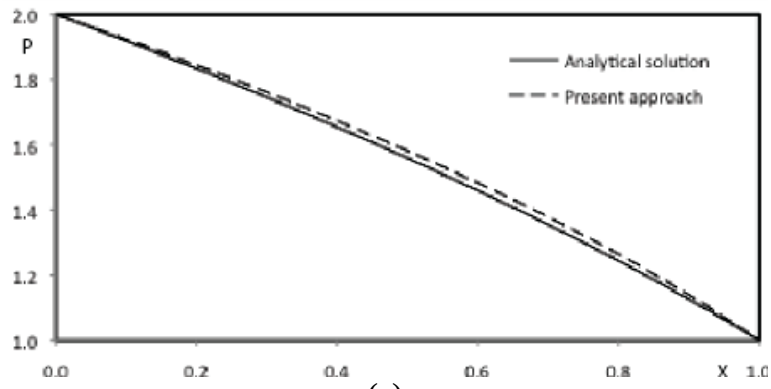
The predicted pressure profiles along the streamwise of the channel is plotted and compared with the analytical solution provided by Arkilic et al, [4] Figs. 2a-2d show the comparisons for *Kn = 0.02, 0.05, 0.1* and *0.15* respectively.



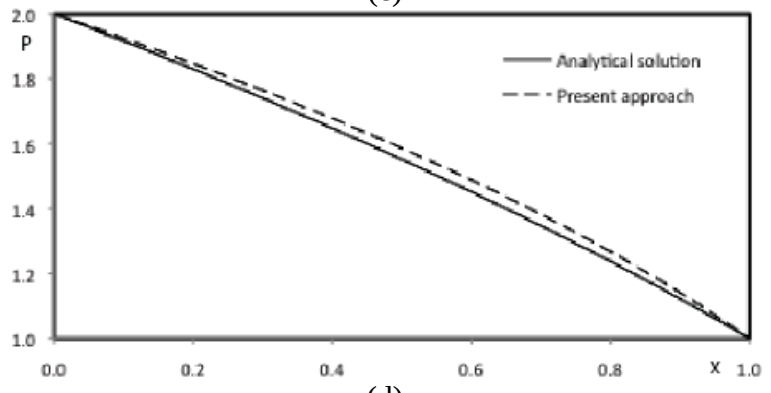
(a)



(b)



(c)



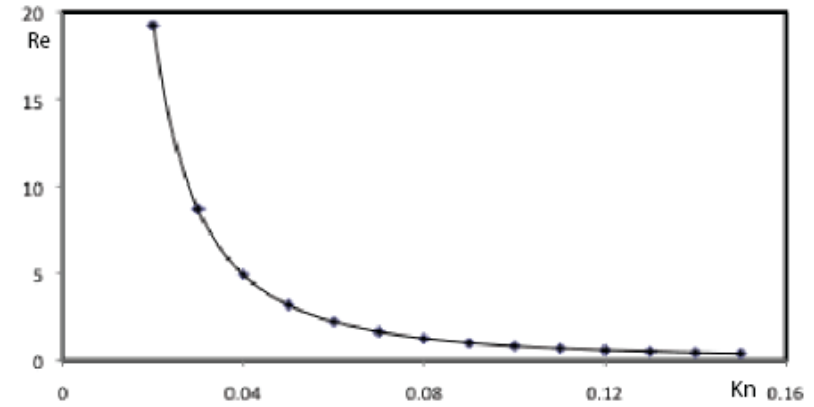
(d)

Figure 2. Pressure profile along the microchannel for (a) *Kn* = 0.02 and (b) *Kn* = 0.05 (c) *Kn* = 0.1

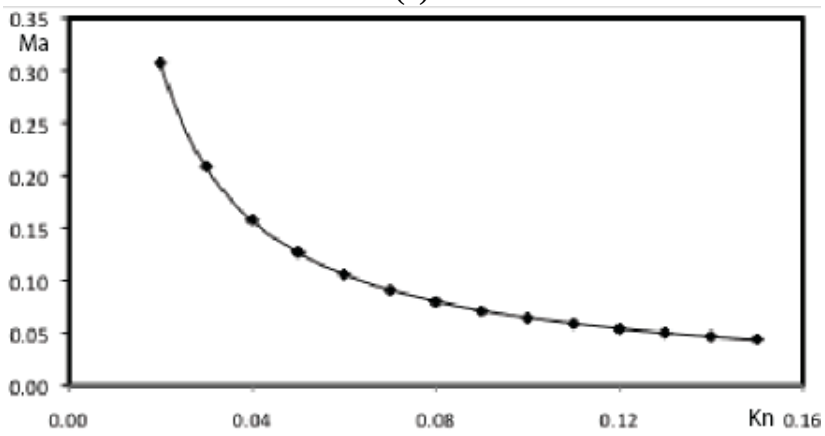
and (d) $Kn = 0.15$

As can be seen from figure 2, a non-linear pressure profile along the microchannel profile can be clearly observed for all Knudsen number values. This non-linearity is due to the compressibility effects and in contrast with the linear variation of incompressible flows. As Kn increases, the non-linearity of pressure becomes less pronounced. This finding is consistent with the results obtained by previous researchers [11], [20], [22], [24] and[25]. However, there is a little deviation for $Kn = 0.15$ can be observed. This is expected because the first order slip velocity model used by Arkilic et al, [4] solution is no longer valid for this Knudsen number while we look at the issue in a more rarefied sense where the molecular dimensions are concerned.

Figures 3a and 3b show the plots of Reynolds and Mach numbers for every simulation of Knudsen number. As can be seen from the figures, both Mach and Reynolds number decrease monotonically as Knudsen number increases.



(a)



(b)

Figure 3. (a) Plots of calculated Reynolds number for every simulation of Knudsen number (b) Plots of calculated Mach number for every simulation of Mach number

5. Conclusion

In this paper, a lattice Boltzmann method based simulation of microscale flow has been carried out, for Knudsen number between 0.02 and 0.15 (slip to transitional regimes). Conventional bounce-back boundary condition together with the inclusion of density dependence relaxation time has been applied into the formulation of LBM. Computation of pressure driven flow in a microchannel correctly predicted the pressure distribution along the channel and agrees well with the analytical solution. Our numerical results confirm the rarefaction`s negation on non-linearity of pressure. Although we use the two-dimensional isothermal model in present study, the approach can

be easily extended to non-isothermal and three-dimensional model. A detailed investigation for non-isothermal microscale flow will be reported in the future.

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Nomenclature

e	Microscopic velocity	u	Velocity
f	Distribution function	U	Centerline velocity at outlet
f^{eq}	Equilibrium distribution function	υ	Viscosity of fluid
H	Characteristic height	ρ	Density
l	Mean free path of particle	τ	Relaxation time
P^*	Pressure distribution		

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