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Simulation of High Knudsen Number Gas Flows in Nanochannels via the Lattice Boltzmann Method

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Abstract. Using a modified Lattice Boltzmann Method (LBM), pressure driven flow through micro and nano channels has been modeled. Based on the improving of the dynamic viscosity, an effective relaxation time formulation is proposed which is able to simulate wide range of Knudsen number, Kn, covering the slip, transition and to some extend the free molecular regimes. The results agree very well with exiting empirical and numerical data.

Introduction

Fluid flow plays a major role in micro and nano devices therefore; it has attracted the interests of the computational fluid dynamic researchers significantly. To categorize flow regimes, a nondimensional number known as the Knudsen number (Kn) is defined. It is the ratio of the molecular mean free path to a flow geometric characteristics length. For $0.01 < Kn < 0.1$, flow can be assumed continuous, but slip velocities appear on solid walls. For the transition regime ($Kn > 0.1$), the continuity assumption and consequently the validity of the Navier Stokes Equations, NSE, is questionable as the size is reduced significantly. In such cases, because of the solid walls effect, the fluid flow behavior depends strongly on the geometry dimensions [1].

the Lattice Boltzmann Method (LBM) is an approach for the flow simulation in small scales. The Lattice Boltzmann Equation (LBE) is a more fundamental equation compared to the NSE, which is valid for all ranges of Knudsen number [5]. Therefore, the LBM can be used to simulate fluid flows in all regimes upon appropriate adjustments [6].

Recently there have been attempts to use the LBM for gaseous flows in slip flow regime but only a few papers can be mentioned for the use of LBM in transition regime [7-13]. To this end, two methods are proposed based on the use of higher order LBM [7-10] and the modification of the mean free path [11-13]. The multi-speed or higher order LBM has been developed to increase the order of accuracy in the discretization of velocity phase space. Although Ansumali, et al. [9] have demonstrated that the high order LBMs have improved current capability but Kim, et al. [10] showed that this method can predict the rarefaction effects only for $Kn = O(0.1)$ and at large Kn, the mass flow rate can not be predicted properly by these methods. Additionally, the high-order LBMs with large numbers of discrete velocities are not numerically stable [14]. On the other hand, the models based on the local mean free path are complicated and can not be used for complex geometries such as porous media.

In this article, by relating the viscosity to the local Kn, a generalized diffusion coefficient is obtained in such a way that wide range of Kn regimes of flow can be simulated more accurately.

The LBM

The continuum Boltzmann equation is a fundamental model for rarefied gases in the kinetic theory [15,16]. Due the complicated nature of the Boltzmann equation [17] Bhatnagar, Gross and Krook [18] proposed a simplified model for LBM known as the BGK-LBM:

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

where $\tau = \lambda / \Delta t$ is the nondimensional relaxation time and f_i^{eq} is the discrete equilibrium distribution function and can be calculated through the Eq. 2 [19].

$$f_i^{eq}(\vec{x},t) = \rho.w_i\left(1+\frac{\vec{u}.\vec{c}_i}{RT}+\frac{\left(\vec{u}.\vec{c}_i\right)^2}{2\left(RT\right)^2}-\frac{\vec{u}.\vec{u}}{2RT}\right)$$
$$w_0 = \frac{4}{9}, w_{i=1,2,3,4} = \frac{1}{9}, w_{i=5,6,7,8} = \frac{1}{36} \quad (2)$$

In the present work, the nine velocity 2D model (D2Q9), is used to discrete momentum space for the present calculations [20]. In this model, the discrete velocity field $\vec{c}_i = (c_{ix}, c_{iy})$ is:

$$\vec{c}_i = \begin{cases} (0,0), & i = 0 \\ (\cos(\frac{i-1}{2}\pi), \sin(\frac{i-1}{2}\pi))c, & i = 1,...,4 \\ \sqrt{2}(\cos(\frac{2i-9}{4}\pi), \sin(\frac{2i-9}{4}\pi))c, & i = 5,...,8 \end{cases} \quad (3)$$

where $c = \Delta x / \Delta t$. Δx and Δt are lattice spacing and time step, respectively. The flow parameters are then calculated in terms of the particle distribution function $f_i(\vec{x},t)$, by:

$$\rho = \sum_{i=0}^{8} f_i \quad , \quad \vec{u} = \frac{1}{\rho}\sum_{i=0}^{8}\vec{c}_i f_i$$
$$P = \rho c_s^{\,2} \quad , \quad c_s^{\,2} = RT = \frac{c^2}{3} \quad (4)$$

where c_s is the lattice speed of sound and P is the pressure. In the standard LBM, the kinematic viscosity υ is shown to be proportional to the relaxation time, as given below and is a constant value.

$$\upsilon = c_s^2 \delta t(\tau - 0.5) \quad (5)$$

In the present work, the slip reflection boundary condition (SRBC) [21] which is a combination of the bounce back and specular boundary conditions is used to predict the slip velocity on solid walls. For example, at the lower boundaries, the unknown particle distribution functions f_2, f_5 and f_6, can be calculated as follows:

$$\begin{bmatrix} f_5(x,0) \\ f_2(x,0) \\ f_6(x,0) \end{bmatrix} = \begin{bmatrix} s & 0 & 1-s \\ 0 & 1 & 0 \\ 1-s & 0 & s \end{bmatrix} \begin{bmatrix} f_7(x+\delta x, \delta y) \\ f_4(x, \delta y) \\ f_8(x-\delta x, \delta y) \end{bmatrix} \quad (6)$$

where $s = 0.5$ is the slip-reflection coefficient on the solid wall.

LBM for high Knudsen number flows

From the Direct Simulation Monte Carlo, DSMC, method and the linearized Boltzmann equation [22], it is evident that the velocity profiles of flow in a channel in the transition and free molecular regimes remain approximately parabolic. But the velocity profile obtained from continuum based relations does not predict the flow rate properly [23]. This is because of the fact that the dynamic viscosity which is related to the diffusion of momentum due to the intermolecular collisions must be modified to consider the diffusion of momentum due to the intermolecular collisions and the collision of molecules with the walls which is the dominant phenomenon in the transition and free molecular regimes [24]. Therefore, a general form of the effective viscosity as a function of the Knudsen number has been proposed [23], which is valid for a wide range of flow regimes.

$$\mu_{eff} = \frac{\mu}{1+2.2Kn} \tag{7}$$

Considering the effective viscosity and density, we have defined a new effective relaxation time in the LBM as follows:

$$\tau_{eff} = 0.5 + \left(\frac{1}{1+2.2Kn} \frac{\rho}{\rho_{eff}} \right) (\tau - 0.5) \tag{8}$$

where $\tau = 0.5 + \sqrt{6/\pi} KnH$ is the nondimensional relaxation time and H is a characteristics length (e.g. height of the micro channel) [25].

Results and discussion

Fully developed pressure driven flows in micro channels with different Knudsen numbers are simulated as a benchmark case for validating present work. In Fig. 1 the nondimensional velocity profiles normalized by local average velocity which is obtained in the transition flow regime for K = 0.1 to 10 is plotted across the channel, where K is $(\sqrt{\pi}/2)Kn$. The corresponding linearized Boltzmann solution is also included [22]. It is seen that the LBM velocity profile and the linearized Boltzmann solution agree quiet well through the Knudsen numbers up to 10. However, a little discrepancy appears very close to the walls. It is because of the fact that the intermolecular forces between fluid molecules and solid walls become important near the walls, in the transition regime [26].

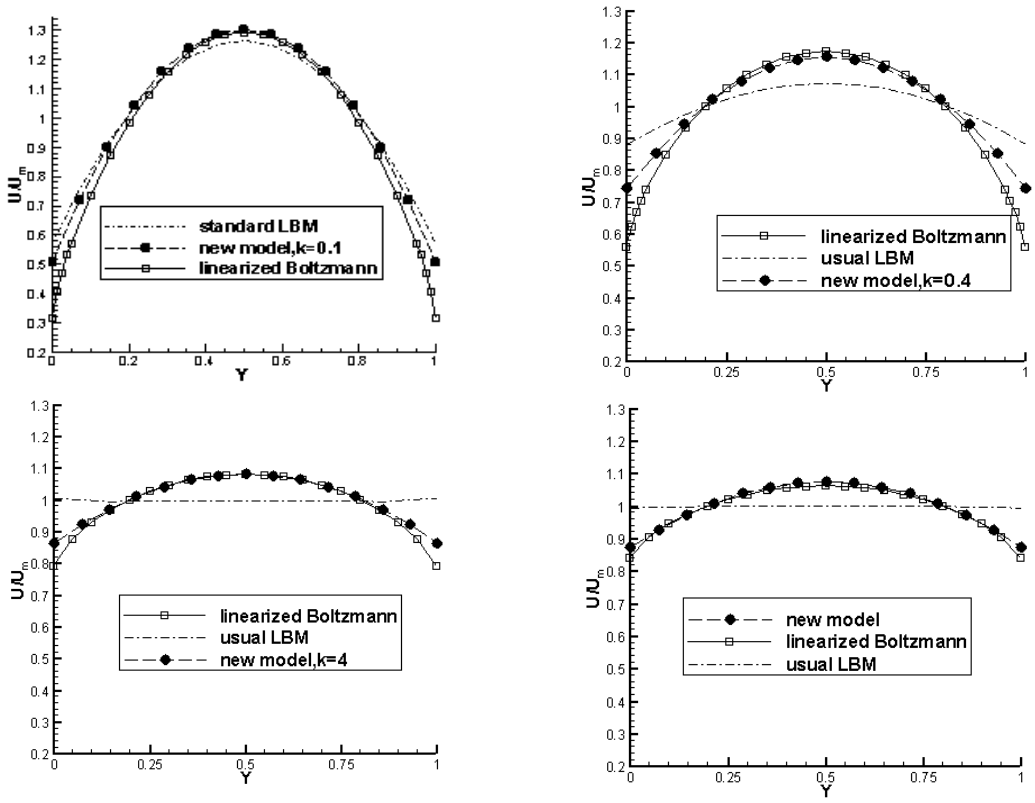

Fig. 1- Normalized velocity distribution across the micro/nano channel

Fig. 2 shows the normalized flow rate through micro/nano channel as a function of the Knudsen number. It can be seen that by increasing the Knudsen number, the flowrate decreases initially and has a minimum value for $Kn \approx 1$, then it increases [27,28]. This phenomenon is called Knudsen minimum effect [29]. Although from the kinetic theory of gases, there is no analytical formula for flow rate in the transition regime, there are two asymptotes for normalized flow rate which is evident in Eq. 9 [16].

$$Q_0 = (6Kn)^{-1} + s + (2s^2 - 1)Kn \quad Kn < 1$$
$$Q_\infty = (1/\sqrt{\pi})\ln(Kn) \quad Kn \to \infty \tag{9}$$

where s = 1.015.

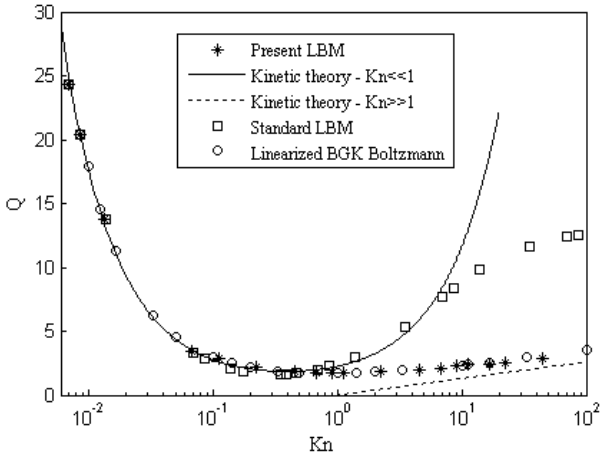

Fig.2- Volumetric flowrate as a function of exit Kn

It can be seen from the figure that our results are in a good agreement with those of the Eq. 19 as well as the linearized Boltzmann method [39]. In Fig. 2, the results of the standard LBM, are also presented. Against the standard LBM, the present results by modifying LBM are accurately compatible with linearized Boltzmann method in the entire transition flow regime. As shown in Fig. 2, the Knudsen minimum effect is captured for $Kn \approx 1$ by using our new model. Noticeably, this interesting agreement is achieved without incorporating any kind of complex and adjustable slip models.

Conclusion

The new LBM is capable of simulating the flow for a wide range of Knudsen numbers including the transition regime. It is shown that the proposed model by modifying the relaxation time in LBM, is able to predict the flow features in micro and nano scales for wide range of Kn, accurately. nondimensional velocity distribution and flow rates are in a good agreement with the exiting analytical data and the well known Knudsen minimum effect in micro and nano channels are achieved for $Kn \approx 1$. These results are obtained without incorporating any kind of adjustable slip models.

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