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Extended application of lattice Boltzmann method to rarefied gas flow in micro-channels

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HIGHLIGHTS

- A lattice Boltzmann model for micro-channel gas flow with Knudsen number up to 10 is proposed.
- Knudsen layer effect on rarefied gas flow with Knudsen number up to 30 is investigated.
- A constant non-dimensional flow rate and linear pressure distribution along the micro-channel are observed for the free molecular flow.

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ABSTRACT

Simulation of rarefied gas flow in micro-channels is of great interest owing to its diverse applications in many engineering fields. In this study, a multiple-relaxation-time lattice Boltzmann (MRT-LB) model with a general second-order slip boundary condition is presented to investigate the behaviour of gas flow with a wide range of Knudsen number in micro-channels. With the aid of a Bosanquet-type effective viscosity, the effective relaxation time is correlated with local Knudsen number (Kn) to account for the varying degree of rarefaction effect. Unlike previous studies, the derived accommodation coefficient r for the combined bounce-back/diffusive reflection (CBBDR) boundary condition is dependent on the local Kn, which allows more flexibility to simulate the slip velocity along the channel walls. When compared with results of other methods, such as linearised Boltzmann equation, experimental data, direct simulation Monte Carlo (DSMC) and Information Preservation DSMC (IP-DSMC), it is found that the LB model is capable of capturing the flow behaviour, including the velocity profile, flow rate, pressure distribution and Knudsen minimum of rarefied gas with Kn up to 10. The effect of Knudsen layer (KL) on the velocity of gas flow with a wide range of Kn is also discussed. It is found that KL effect is negligible in the continuum flow and y-independent in the free molecular flow, while in the intermediate range, especially in transition flow, KL effect is significant and particular efforts should be made to capture this effect.

1. Introduction

Studies on rarefied gaseous flow in micro-channels have drawn intense interests in recent years, because of its fundamental nature and diverse application in the aerodynamics, heat transfer, nanotechnology, microelectromechanical systems (MEMS), shale gas [1,2] and other areas. Lattice Boltzmann method (LBM) has shown its superiority to delineate the rarefied gas flow, due to its kinetic origin and computational efficiency. Its success in modelling slip gas flow has motivated

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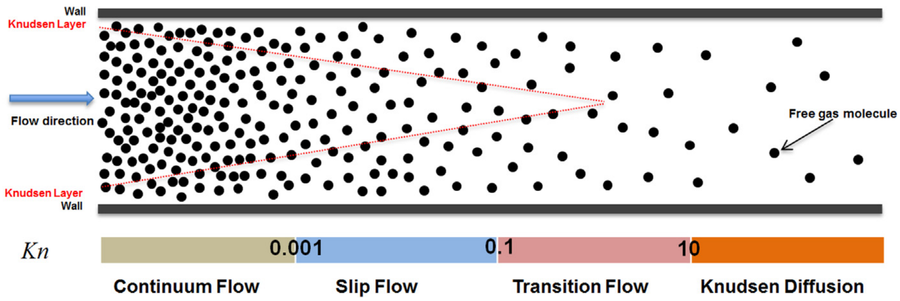

Fig. 1. Different flow regimes in a long micro-channel under a given pressure difference. Black dots represent the free gas molecules in the micro-channel; red dash lines represent the increasing thickness of Knudsen layer towards outlet. This is a schematic diagram under the assumption of infinitely long micro-channel and high pressure difference between inlet and outlet. Note that the height of the micro-channel is magnified.

the research efforts to extend the application of LBM to the transition flow regime. Although a couple of lattice Boltzmann (LB) models have been developed for this purpose [3–5], no single one has demonstrated its universal acceptance to capture the rarefaction effect of transition flow in micro-channels.

It was first observed experimentally by Knudsen [6] that gas flow through tubes deviates from the Poiseuille flow under decreasing pressure. This phenomenon was explained by the fact that the gas molecules under low pressure are rarefied and not dense enough to be considered as a continuum medium. For the rarefied gas, the continuum assumption breaks down and hence the discrete nature of gas molecules cannot be ignored. In order to characterise this rarefaction effect, Knudsen number, Kn was introduced and defined as the ratio of mean free path, λ of the gas molecules to the characteristic length of flow paths, H as

$$Kn = \frac{\lambda}{H}. \tag{1}$$

Gas flow in micro-channels is divided into four flow regimes according to the value of Knudsen number: continuum flow ($Kn < 0.001$), slip flow ($0.001 < Kn < 0.1$), transition flow ($0.1 < Kn < 10$) and free molecular flow ($Kn > 10$). Compared with the height of channel H, mean free path of gas molecules in the continuum flow is so small that gas can be considered as a continuous medium, thus classical Navier–Stokes equations can be applied. In the free molecular flow, the mean free path is very large and collision between gas molecules and channel walls is dominant. Gas molecules move independently and intermolecular collision is insignificant. Gas flow in this regime can be described by Knudsen diffusion. For the intermediate range of Knudsen number, flow is further divided into slip flow and transition flow. The slip flow is usually modelled by the Navier–Stokes (N–S) equations with first-order slip boundary conditions while the transition flow still lacks clear understanding. Variation of flow regimes in a long micro-channel under high pressure difference is depicted in Fig. 1, and detailed description of flow regimes can be referred to Yuan et al. [7]. Due to the limited understanding, particular emphasis of various models is usually placed on the transition flow regime.

In order to model the rarefied gas flow, classical N–S equations are corrected with different slip boundary conditions. Arkilic et al. [8] successfully used perturbation expansion of the N–S equations with a first-order correction of wall slip to predict the increased mass rate of slip flow in micro-channels. This work was further extended by Dongari et al. [9] who provided solution to the N–S equations with a second-order slip boundary condition at walls and found that the solution roughly agrees with Boltzmann's solution up to Kn around 5. Alternatively, Brenner [10,11] proposed the idea of extended N–S equations. The key idea is that there is density-gradient-driven diffusion in addition to the pressure-driven convection for rarefied gas flow in micro-channels; the former diffusion contributes to extra flow rate. Using this extended N–S equations, Dongari et al. [12] successfully captured the enhanced mass flow rate in micro-channels. This is similar to the perspective of dusty gas model (DGM), which considers that the molecular diffusion, Knudsen diffusion and viscous flow coexist in the porous media and contribute to the total flux by a linear combination of these mechanisms [13]. The linear combination approximately averages the contribution from each mechanism to the total flow rate. Recently, DGM is widely employed by reservoir engineers to derive the apparent gas permeability for a single capillary of tight rocks like shale [14–16]. This application, however, is quite questionable for flow in a single channel/ capillary. It is seen from Fig. 1 that the degree of rarefaction effect increases from the inlet (with high pressure and low Kn) to the outlet (with low pressure and high Kn) of a long micro-channel. Irrespective of flow regimes that may be encountered along a long micro-channel, the flow rate is determined by the flow regime at the outlet, rather than all regimes encountered. An additional problem with these N–S equations and DMG is that the change of kinetic properties, such as the viscosity, is ignored for the rarefied gas.

As the basic model originated from kinetic theory, Boltzmann equation (BE) was first put forward by Boltzmann [17] to describe the rarefied gas dynamics. In the equation, gas is considered as composing of interacting particles characterised with distribution functions; the macroscopic behaviour of gas is statistically calculated through the evolution of distribution functions [18]. In comparison with N–S equations, it can be seen that BE can be applied to the non-continuous medium, such as rarefied gas flows. Solution of the BE, however, can be very complicated because of its nonlinearity and the requirement of integration of a function comprising six independent variables [19]. When the average speed and temperature of gas exhibit