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A novel modified lattice Boltzmann method for simulation of gas flows in wide range of Knudsen number ☆

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ABSTRACT

To cover a wide range of the flow regimes, a new relaxation time formulation by considering the rarefaction effect and the effective dynamic viscosity has been obtained. By using the modified lattice Boltzmann method (LBM), pressure driven flow through micro and nano channels has been modeled for wide range of Knudsen number, Kn, covering the slip, transition and to some extent the free molecular regimes. The results agree very well with existing empirical and numerical data. The velocity profile was predicted as well as the volumetric flow rate and for the first time, the well known Knudsen minimum effect has been captured about Kn = 1.

1. 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 characteristic length. For $0.01 < Kn < 0.1$, flow can be assumed as 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].

Molecular based methods such as Molecular Dynamics (MD) and Direct Simulation Monte Carlo (DSMC) methods [2] maybe used to model micro and nano flows for a wide range of the Knudsen numbers [3,4]. However, the computational cost of these molecular based methods is prohibitively high such that they cannot be used for practical fluid flow simulations in micro and nano scales except for free molecular regimes.

A midway approach for the flow simulation in small scales is the lattice Boltzmann method (LBM). Because the LBM is a mesoscopic method which can be considered as a particle based method and at the same time is independent of the actual number of molecules, it requires less computational resources for low Kn flows. Moreover 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 [7–13] but only a few papers can be mentioned for the use of LBM in transition regime [14–20]. To this end, two methods are proposed based on the use of higher order LBM [14–17] and the modification of the mean free path [17–20]. 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. [16] have demonstrated that the high order LBMs have improved current capability, Kim et al. [17] showed that this method can predict the rarefaction effects only for $Kn = O(0.1)$and at large Kn, the mass flow rate cannot be predicted properly by these methods. Additionally, the high-order LBMs with large numbers of discrete velocities are not numerically stable [21].

On the other hand, for high Kn flows that the mean free path, λ, becomes comparable with the channel dimensions, the wall boundaries reduce the local mean free path. Therefore, by using a geometry dependent local mean free path, Tang et al. [20] captured the nonlinear high order rarefaction phenomena, but this local mean free path is complicated and cannot 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.

2. The LBM

The continuum Boltzmann equation is a fundamental model for rarefied gases in the kinetic theory [22,23]. It is an integro-differential equation in which the collective behavior of molecules in a system is used to simulate the continuum mechanics of the system. The Boltzmann equation is written as follows:

$$\partial_t f + \left(\vec{\xi}.\nabla\right) f = Q(f, f') \tag{1}$$

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