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Lattice Boltzmann method for rarefied channel flows with heat transfer

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ABSTRACT

A thermal lattice Boltzmann method (TLBM) is presented for the analysis of fluid flow and heat transfer in two-dimensional channels with non-continuum effects. The relaxation times (τ_f, τ_g) are linked to the Knudsen number which accounts for the rarefaction that can be present at micro geometries or at low density conditions. The TLBM used here employs inlet/outlet boundary conditions to generate a forced convection problem where the calculation of equilibrium distributions at the wall surfaces are modified to incorporate the velocity slip and temperature jump conditions. Numerical simulations are obtained for thermal micro-Couette and thermal micro-Poiseuille channel flows and the effect of the Knudsen number on the velocity and temperature profile is investigated.

1. Introduction

The lattice Boltzmann method is a kinetic method based on the particle distribution function and during the past few years it has gained the attention of many researchers whom investigated the applicability of LBM for simulation of microscale flows (Table 1).

Nie et al. [1] applied the LBM method for compressible flow in microchannels and micro-cavities and they have observed that LBM can capture behaviors such as velocity slip, nonlinear pressure distribution along the channel and dependence of mass flow rate on Knudsen number. In their study they have used a D2Q9 model on a two-dimensional, square lattice. They used a modified relaxation time in order to include the dependence of viscosity on density for compressible flows. They defined the mean free path as a function of viscosity and density multiplied with a coefficient that was determined by comparing simulation results with microchannel experiments. Bounce-back wall boundary conditions were used for the particle distribution functions at the top and bottom plates. This boundary condition results in a non-slip velocity in the continuum regime; however, the results have shown that when *Kn* is large, a mean slip velocity on wall boundary can be achieved. This was owed to the kinetic nature of the LBM.

Lim et al. [2] used specular reflection and a second order extrapolation scheme for gas interaction with surfaces in their LBM simulations. The non-linear pressure distribution, increase of slip velocity along the channel, and radial velocity profile obtained were in agreement with analytical results [3]. Their result for the slip flow regime was in good agreement with experimental data of Pong et al. [4] for pressure distribution along the microchannel. However, it was observed that using different boundary treatment has little influence on pressure distribution, though the effect on slip velocity on the wall surfaces is significant. Further investigation has shown that the mass flow rate and the overall average velocity were in perfect agreement with Arkilic's analytical solution [3] and the mass flow rate was found to be insensitive to the boundary treatment on the wall surfaces.

Tang et al. [5] has combined the bounce-back boundary condition [1] with the specular reflection boundary condition [6] in order to accurately capture the momentum exchange and friction drag between the wall surface and the gas in microflows. They have defined a reflection coefficient r_b for which $r_b = 1$ corresponds to pure bounce-back reflection and $r_b = 0$ to pure specular reflection. Using a value of $r_b = 0.7$ they have successfully matched the mass flow rate and the non-linear pressure variation observed in the experiments by Shih et al. [7] for $Kn = 0.16$. Recently, the authors extended their model to 3D by using a $D3Q15$ lattice model [8]. Their LBM results for nonlinear pressure profiles were in good agreement with the 3D analytical model of Aubert et al. [9].

Shen et al. [10] has extended the work of Nie et al. [1] and compared the results for velocity and pressure distributions for microchannels with the results obtained with DSMC, IP, and slip NS methods. In their LBM simulations they have used bounce-back boundary condition on the walls and the extrapolation scheme [11] at the inlet and exit of the channel. In their definition of the mean free path, they use a coefficient whose value ($a = 0.388$) is

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Table 1
Lattice Boltzmann method for gas flow in microchannels in literature.

#	Author	Year	*Kn*	Boundary condition
1	Nie et al. [1]	2002	$Kn = \alpha\tau/\rho H$	Bounce back
2	Lim et al. [2]	2002	$Kn = \delta x(\tau + 0.5)/H(P_o/P)$	Specular reflection and extrapolation scheme
3	Tang et al. [5]	2003	$Kn = \alpha\tau/\rho H$	
4	Shen et al. [10]	2004	$Kn = \alpha\tau/\rho H$	Bounce back
5	Lee et al. [12]	2005	$Kn = \delta x\tau/H(P_o/P)$	Wall equilibrium
6	Zhang et al. [15]	2005	$Kn = \alpha\tau/\rho H$	Maxwellian scattering
7	Zhou et al. [20]	2006	$Kn = \alpha\tau/\rho H$	Bounce back

determined from the best match of the results with the experiments. The flow rate prediction of LBM was observed to be in good agreement with other methods for $Kn = 0.0194, 0.194$, and 0.388. The velocity profile and the pressure distribution results were found to be in good agreement with the results of other methods for $Kn = 0.0194$ however for $Kn = 0.194$ and 0.388 the LBM velocity profile and pressure variation were observed to deviate from the results of DSMC and IP. Depending on these results the authors have concluded that the version of LBM proposed by Nie et al. [1] shows feasibility to simulate MEMS gas flow in continuum and slip flow regimes but not in the transition regime where the Knudsen number is large.

Lee et al. [12] proposed a second order definition of Knudsen number and a wall equilibrium boundary condition for LBM to simulate gas flows in a microchannel. They tested their method for gas flow in a periodic microchannel with constant external pressure gradient. The normalized slip velocity was found to be in excellent agreement with the analytical prediction of Arkilic [3] for $Kn < 0.1$. They validated their proposed LBM method by comparing their results for normalized streamwise velocity profile with those of the linearized Boltzmann equation [13] and the DSMC methods [14] for $Kn = 0.1$. The LBM solution was found to be in excellent agreement with the others. Their model was also tested for gas flow in a microchannel with constant pressures at inlet and exit. It was shown that the slip velocity is in good agreement with Arkilic's prediction [3]. They have concluded that their proposed method for the definition of Knudsen number and the wall equilibrium boundary condition is more physically meaningful compared to previous versions of LBM simulations for microchannel flow [1,2].

Zhang et al. [15] showed that LBM can predict the correct trend of mass flow rate as the Knudsen number increases along the microchannel and captures the ''Knudsen minimum'' phenomena, which was observed previously in experiments [16]. A slip boundary condition was proposed by adopting the Maxwellian scattering kernel to describe gas surface interactions. Their proposed boundary condition requires the assignment of a constant for the accommodation coefficient.

The Knudsen paradox was also captured by Toschi and Succi [17] for flow in a rectangular duct where the flow was driven by a volumetric force along the streamwise direction. In their simulations they compared the performance of the bounce back boundary condition [11] and the kinetic boundary condition proposed by Ansumali and Karlin [18] in the rarefaction range $10^{-3} < Kn < 30$ and at a fixed Mach number $Ma = 0.03$. Being independent from the boundary condition at the wall surfaces, Toschi and Succi have proposed that every LBM simulation at finite *Kn* regime should take care of the momentum transfer along the direction orthogonal to the boundaries. In order to achieve this, they proposed a virtual wall collision (VWC) model that should be implemented at every lattice site in the flow domain. Their simulations have shown that with VWC model the results for the mass flux was in good agreement with the analytical prediction of Cercignani [19]. The bounce back boundary condition has shown to be incapable of predicting the correct wall slip velocity in the high Knudsen number regime. They have concluded that the LBM method using the kinetic wall boundary conditions of Ansumali and Karlin [18] combined with their VWC method [17] can capture continuum and non-continuum effects of microchannel flow.

Lattice Boltzmann method has been introduced to the scientific community as a new alternative numerical method that can solve for flows with complex physics [21,22] however there are still areas that need to be studied in order to obtain a well-established numerical method that covers a wide range of engineering applications. One aspect of this improvement is the solution of flows with heat transfer [23,24]. In an effort to obtain a thermal lattice Boltzmann method (TLBM), a variety of techniques were proposed in the literature, namely the multi-speed approach, the passive-scalar approach and the double populations approach. The model developed by He et al. [25] has gained the most popularity because it was more stable and it had the capability to solve for viscous dissipation and compression work. In this model, the thermal lattice Boltzmann equation was derived by discretizing the Boltzmann equation for the internal energy distribution. As a result, thermal energy and heat flux were able to be obtained by taking the kinetic moments of the thermal energy distribution function.

The method proposed by He et al. [25] was accepted by many researchers and it was successfully applied to solve for various kinds of fluid flow problems with heat transfer. Dixit and Babu [26] used this model to simulate natural convection of a Boussinesq fluid in a square cavity. It was demonstrated that for high Rayleigh numbers the TLBM results agreed well with other benchmark numerical simulations. Tang et al. [27] proposed boundary conditions to improve the same model in order to solve for two-dimensional Poiseuille and Couette flow and verified the TLBM results with Finite Volume Method and analytical solutions at various wall boundary conditions. D'Orazio and Succi [28] introduced a counter-slip internal energy boundary condition for the TLBM model and obtained satisfactory results for hydrodynamically and thermally developed channel flows heated at the inlet. In their simulations, the TLBM was able to capture the effect of viscous dissipation which was tested for thermal Couette flow at various Brinkmann numbers.

There have been a couple of studies that aimed to implement the TLBM in fluid flow and heat transfer in complex geometries. Huang et al. [29] solved the natural convection in a concentric annulus involving circular solid boundaries. The curved non-slip wall boundary treatment for isothermal LBM [30] was extended to treat the thermal curved solid boundary in the two-population TLBM computations. Chen et al. [31] applied the same boundary condition for two-dimensional solutions of backward-facing step flows with inclined plates positioned along the flow field at various angles. Gokaltun and Dulikravich [32] verified the TLBM solutions for a constricted channel flow against FEM solutions for velocity and thermal fields.

Heat transfer in microscales is a major issue in analysis and design of computer chips and cooling of electronic equipments. Due to its kinetic nature, LBM can be an important tool in the study