Capture the rarefaction effect in microchannels using the TRT-LBM model

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Abstract. The rarefaction effect of gas flow in microchannels has been received particular attention in recent years. This paper employs TRT-LBM coupled with the effective viscosity and slip velocity boundary condition in the prediction of rarefaction in microchannels in rarefied air. The result shows that the present TRT-LBM model can satisfactorily capture the rarefaction effect in microchannels compared with the results of DSMC and MRT-LBM models.

1. Introduction
Recently, the lattice Boltzmann method (LBM) has been developed as an alternative numerical scheme for fluid flow simulation especially gas flow in microchannels [1-3]. As the gas becomes rarefied in microchannels, the rarefaction effect tends to dominate and the molecule mean free path could be affected by the solid wall. This situation leads to the formation of the Knudsen layer, which the effective viscosity has been proposed [4-7].

The single relaxation time lattice Boltzmann method (SRT-LBM) has been applied to microchannel flows in many studies. However, as pointed out in some recent works [8][9], the slip velocity depends on the relaxation time in SRT-LBM model, which may vary with lattice number at a given Kn. The multiple relaxation time lattice Boltzmann method (MRT-LBM) can avoid this problem by implementing several relaxation times. The two relaxation time lattice Boltzmann method (TRT-LBM) can also resolve the unphysical slip velocity by providing two relaxation times [9][10]. In this paper, the TRT-LBM model is used to capture the rarefaction effect in microchannels.

The outline of this paper is as follows, in section 2, the TRT-LBM process is given, and the effective viscosity and boundary conditions are determined. In section 3, the results of the present TRT-LBM are compared with the data of DSMC[6].

2. TRT-LBM

2.1. Process of TRT-LBM
The TRT-LBM model can be written as:

\[ f_i(x + \delta_x, t + \delta_t) = f_i(x, t) - \frac{(f_i^s - \bar{f}_i^{eq})}{\tau_s} - \frac{(f_i^a - \bar{f}_i^{eq})}{\tau_a}, \quad i = 0, 1, 2...N \]

(1)

where the subscript \( i \) denotes the discrete direction, \( N \) is the number of discrete velocity, the D2Q9 model is used in the TRT-LBM method and \( N=8 \), \( \delta_x \) and \( \delta_t \) are lattice spacing and lattice time step, which are usually both set as 1. Superscripts \( s \) and \( a \) indicate the symmetrical and antisymmetrical
parts of the distribution function. \( \tau_s \) is relaxation time related to viscosity, \( \tau_a \) is relaxation time related to energy flux. The symmetrical and antisymmetrical distribution functions can be given as follows:

\[
f_i^s = \frac{(f_i + f_{-i})}{2}, f_i^{eq} = \frac{(f_i^{eq} + f_{-i}^{eq})}{2}, f_i^a = \frac{(f_i^{eq} - f_{-i}^{eq})}{2} \quad (2)
\]

where \( -i \) is the direction opposite to \( i \). The local equilibrium distribution function \( f_i^{eq} \) can be defined as:

\[
f_i^{eq} = \omega_i \rho \left[ 1 + \frac{c_i \cdot u}{c_i^2} + \frac{(c_i \cdot u)^2}{2c_i^4} - \frac{u^2}{2c_i^2} \right]
\]

where \( \omega_i \) are weight factors, \( c_i \) is the lattice sound speed, \( u \) is the macroscopic flow velocity.

\( c_s = c / \sqrt{3}, c = \delta_s / \delta_i \).

The macroscopic variables such as density \( \rho \), macroscopic flow velocity \( u \) and macroscopic pressure \( P \) can be evaluated as follows:

\[
\rho = \sum_i f_i^s, \quad u = (1/\rho) \sum_i f_i^s, \quad P = \rho \cdot c_s^2
\]

The viscosity relaxation time \( \tau_v \) is written as:

\[
\tau_v = 0.5 + \mu / (P \cdot \delta_i)
\]

2.2. Effective viscosity

Stops\[4\] firstly derived a correction function \( \psi(Kn) \) to the mean free path for gas flows confined between two infinite parallel walls:

\[
\lambda_e = \lambda \psi(Kn)
\]

where \( \lambda \) and \( Kn \) are still the conventional mean free path and Knudsen number. The function \( \psi(Kn) \) is very complicated and difficult for application. For simplicity, Guo et al.\[5\] approximated Stop’s function with:

\[
\psi(Kn) = \frac{2}{\pi} \arctan(\sqrt{2}Kn^{-3/4})
\]

Beskok and Karniadakis \[6\] proposed a Bosanquet type expression of effective viscosity:

\[
\mu_e = \mu / (1 + aKn)
\]

where \( a \) is constant, and \( a=2.2 \) is used for microchannels of length to width ratio \( L/H=20\)[6]. Considering the size of microchannels in this paper, the effective viscosity of equation (8) is used and \( a=2\)[7]:

\[
\tau_v = 0.5 + \sqrt{\frac{\pi}{16}} \frac{Kn}{1 + 2Kn} N_{Ht}
\]

where \( N_{Ht} \) is the number of lattice in characteristic length direction.

2.3. Boundary conditions

In rarefied gas flow, the second order slip velocity model is used[11]:

\[
u_s - U_0 = C_1 \frac{\partial u}{\partial y}_{wall} - C_2 \frac{\sigma}{\sigma + 1} \frac{\partial^2 u}{\partial y^2}_{wall}, \quad C_1 = \frac{2 - \sigma}{\sigma + 1}(1 - 0.1817 \sigma), \quad C_2 = \frac{1}{\pi} + \frac{1}{2}
\]

where \( C_1 \) and \( C_2 \) are slip coefficients, \( \sigma \) is the accommodation coefficient, in this paper, the wall boundary is fully diffusive \( \sigma=1 \). The analytical expression of equation (10) can be written as:

\[
u_s - U_0 = (4C_1 Kn_e + 8C_2 Kn_e^2) \frac{H^2 \sqrt{P}}{8 \mu}, \quad Kn_e = \frac{\lambda_e}{H}
\]

In LBM studies, there are three common schemes of slide wall boundary conditions: the bounce back condition (BB)[1]; the combined bounce back and specular reflection boundary condition
(CBBSR)[2]; the discrete Maxwellian boundary condition (DMBC)[3]. Although BB boundary is usually used for no-slip velocity gas flow, it has been demonstrated that BB boundary generates a slip velocity at the wall, which is a function of relaxation times[12]:

\[
u_s = \frac{1}{4} \frac{8 \tau_q - 1}{2 \tau_v - 1} \frac{\nabla P}{\rho}
\]

where \(\tau_q = \tau_v\) and \(\tau_v = \tau_q\) are the relaxation times for viscosity and energy fluxes. The second slip velocity can be achieved by equations (11)(12):

\[
\tau_v = \left[ \frac{\sqrt{6\pi H(C_1 + 2C_2 Kn)}}{8} \right] + \frac{8 \tau_s - 1}{16 \tau_s - 8}
\]

As for the open pressure boundary condition, the extrapolation method is used in the present model.

3. Numerical results

In this section, the TRT-LBM model is compared with DSMC[6] and MRT-LBM[8]. The length to width ratio of the channel is \(L/H=20\), and the inlet to outlet pressure ratio is \(P_{\text{in}}/P_{\text{out}}=2.28\), the inlet and outlet pressures are \(P_{\text{in}}\) and \(P_{\text{out}}\), \(Kn\) at the channel outlet is 0.2. The lattice size used in the simulation is 400×20. It should be noted that MRT-LBM[8] contained the first order, 1.5 order and second order slip models. Also the effective viscosity employed in their models is equation (7). Here, the MRT-LBM results of the second order slip model are applied for comparison. Figure 2 shows the streamwise velocity profiles of the channel flow at the average \(Kn=0.1\sim10\). The velocity and distance are normalized by the mean velocity \(U_{\text{mean}} = \int u(y)dy/H\) and the width \(H\) of the channel.

![Figure 1. Streamwise velocity profile comparisons at the outlet of microchannel.](image-url)
In figure 1, as Kn increases, the rarefaction effect grows, the cure of streamwise velocity profile becomes flat. At Kn=0.1, the results of TRT-LBM and MRT-LBM both agree well with those of DSMC. At Kn=1, MRT-LBM overestimates the slip velocity, and the non-dimensional center velocity is much smaller than that of DSMC, however, TRT-LBM can still match the results of DSMC very well. At Kn=10, MRT-LBM shows significant deviations from DSMC and TRT-LBM, while TRT-LBM can still predict velocity profile well. It should be noted that, the difference of TRT-LBM and MRT-LBM is mainly the effective viscosity. Next, this paper gives simulation of TRT-LBM with equation (7). The result of velocity profiles is shown in figure 2. The results of TRT-LBM agree very well with those of MRT-LBM. On the one hand, TRT-LBM can provide the accuracy nearly the same as MRT-LBM in prediction of rarefaction effect in microchannels. One the other hand, for this case, in the LBM model, the effective viscosity[6] plays better performance than that of Guo et al.[5].

The accuracy of the model in prediction of mass flow rate through microchannels is shown in figure 3. The mass flow rate $M^*$ is normalized[11]:

$$M^* = \sum_{y=0}^{H} \rho u(y) \left[ (P_{in} - P_{out}) H^2 / L \sqrt{2RT} \right]$$

(14)

As can be seen, the results of TRT-LBM agree well with those of MRT-LBM at $Kn<0.1$, however, the deviation becomes larger as $Kn>0.1$. As $Kn$ increases, MRT-LBM overestimates the mass flow rate. On the other hand, the agreement between TRT-LBM and DSMC is excellent up to $Kn=5$, and at $Kn>5$, the prediction of mass flow rate of TRT-LBM is a little smaller than that of DSMC. Meanwhile, MRT-LBM captures the Knudsen minimum phenomenon at $Kn=0.7$, the results of DSMC show the Knudsen minimum phenomenon at $Kn=1$, and for TRT-LBM, the Knudsen minimum phenomenon occurs at about $Kn=1.5$.

![Figure 2. Comparison of TRT-LBM and MRT-LBM with the same effective viscosity.](image1)

![Figure 3. Normalized mass flow rate at the average Kn.](image2)

4. Conclusions
In this paper, a TRT-LBM model for gas flow in microchannels is proposed. By the effective viscosity, the results of the present TRT-LBM agree well with those of DSMC[6]. The present model is better than MRT-LBM[8], especially when $Kn$ is up to 10, and captures the Knudsen minimum phenomenon at about $Kn=1.5$. By using the same effective viscosity, it illustrates that the accuracies of TRT-LBM and MRT-LBM are almost the same, while TRT-LBM keeps advantages such as simple algorithm and low computational cost. The TRT-LBM model with effective viscosity in this paper has successfully captured the rarefaction effect in microchannels.

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