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# Two relaxation time lattice Boltzmann model for rarefied gas flows

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## HIGHLIGHTS

- We simulate a micro/nano-channel flow using a two relaxation time lattice Boltzmann model.
- Consistent relaxation times are defined for a micro/nano-channel flow.
- We study the stability of the two relaxation time model and single relaxation time model.
- Two relaxation time model can fix the deficiencies of the single relaxation time model.

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ABSTRACT

In this paper, the lattice Boltzmann equation (LBE) with two relaxation times (TRT) is implemented in order to study gaseous flow through a long micro/nano-channel. A new relation is introduced for the reflection factor in the bounce-back/specular reflection (BSR) boundary condition based on the analytical solution of the Navier–Stokes equations. The focus of the present study is on comparing TRT with the other LBE models called multiple relaxation times (MRT) and single relaxation time (SRT) in simulation of rarefied gas flows. After a stability analysis for the TRT and SRT models, the numerical results are presented and validated by the analytical solution of the Navier–Stokes equations with slip boundary condition, direct simulation of Monte Carlo (DSMC) and information preservation (IP) method. The effect of various gases on flow behavior is also investigated by using the variable hard sphere (VHS) model through the symmetrical relaxation time.



## 1. Introduction

In the last two decades, the rapid growth of micro electro mechanical systems (MEMS) requires experimental and numerical studies. Due to the small dimensions of micro devices, performing experimental studies is usually an expensive procedure. Therefore, the numerical study of micro/nano-scale flows has been receiving considerable attention.

The most important dimensionless parameter in micro/nano-scale gas flows is the Knudsen number, which is defined as [1]:

$$Kn = \lambda/H \tag{1}$$

where $\lambda$ is the mean free path of gas and $H$ is a characteristic length. In simulation of a micro/nano-channel flow by using the lattice Boltzmann method (LBM), $H$ is equal to the number of grids in the width of the channel. Since in micro/nano devices, $H$ and $\lambda$ have the same order of magnitude, the Knudsen number usually has a large value. Based on the Knudsen number, the

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flow regime can be categorized into four groups: continuum flow ($Kn < 0.001$), slip flow ($0.001 < Kn < 0.1$), transition flow ($0.1 < Kn < 10$), and free molecular flow ($Kn > 10$) [2]. It has been demonstrated that Navier–Stokes equations with slip boundary condition can be applied to gases in the slip flow regime. For the transition flow regime, one should use some other methods such as direct simulation of Monte Carlo (DSMC) or solve the original Boltzmann equation. The DSMC method is directly involved with the number of molecules in the domain. Consequently, the computational effort is usually an important parameter in this method [3]. Recently, LBM, which is another particle based method, has opened a new way in modeling of micro/nano gas flows. In the LBM, the number of distributed particles is only related to the grid size and it is not dependent on the number of molecules in the domain. Therefore, it is computationally less expensive than the DSMC method.

The single relaxation time lattice Boltzmann equation (SRT-LBE) has been applied to micro-channel gas flows in various studies [2–5]. In most of these works mainly the slip flow regime is investigated. Also, Shokouhmand and Isfahani [6] defined a new relation for the relaxation time in the SRT-LBE by using the effective viscosity proposed by Karniadakis et al. [7]. They showed that this relation can improve the prediction of velocity profiles in the transition flow regime. Recently, Liu and Guo [8] introduced an effective bounce back and specular reflection (BSR) boundary condition for the SRT-LBE. They reported that this model can satisfactorily predict the flow behavior with moderate Knudsen numbers. However, their relation is different from theoretical analysis and it is adjusted in order to match the correct slip velocity. Furthermore, this relation depends on the grid size, which is a limitation of the SRT-LBE. Verhaeghe et al. [9] showed that the multiple relaxation time lattice Boltzmann equation (MRT-LBE) can fix the deficiencies of the SRT model by employing several relaxation times. Guo et al. [10] studied the relaxation parameters involved in the MRT-LBE and proposed a relation for the relaxation parameter related to the energy fluxes using a second order slip velocity model. Also, Xu and Guo [11] investigated the effect of different parameters such as aspect ratio and rarefaction on pressure distribution by using the MRT-LBE. On the other hand, several attempts have been done in order to study micro/nano gas flows by using other methods: Ejtehadi et al. [12] studied different gas structures using the DSMC method. They reported the main effective parameters on slip velocity and temperature jump in a micro/nano Couette flow. Roohi and Darbandi [13] obtained an effective viscosity coefficient according to the information preservation (IP) method and imposed it on the Navier–Stokes equations. They demonstrated that by using this new viscosity coefficient, the Navier–Stokes equations can be used to predict the flow behavior at $0.1 < Kn < 0.5$ accurately. The effect of rarefaction and compressibility on micro/nano-scale gas flows is also investigated by using the Burnett equations and DSMC method in Refs. [14,15].

In the present work, the lattice Boltzmann method with two relaxation times (TRT) is implemented in order to study pressure driven gas flow through a long micro/nano-channel. In some of the previous studies it is reported that SRT-LBE is unable to predict the flow behavior at large Knudsen numbers because of the artifacts existing in this model. In other words, in the SRT model, the relaxation parameter linearly depends on the Knudsen number. Therefore, as the Knudsen number increases, the unphysical slip velocity, which is a function of the relaxation parameter, is no longer negligible. One solution for the mentioned problem is to decrease the number of grids for high Knudsen number flows, but this may impair the grid independency of results. It has been demonstrated that MRT-LBE can fix this problem by implementing several relaxation parameters. However, due to computational effort and loss of simplicity, which are the main features of LBE, this model is not as popular as SRT-LBE. Since the TRT model provides two relaxation times, it seems that this method is more efficient in modeling of micro/nano-scale gas flows. We aim to demonstrate that TRT-LBE can operate as efficiently as MRT-LBE in micro/nano gas flow simulations, while it is as simple as SRT-LBE. Also, a modified symmetrical relaxation time is introduced in order to consider the effect of gas structures on flow behavior.

## 2. Physical model

The considered problem is an isothermal pressure driven gas flow in a two dimensional micro/nano-channel. The ratio of length to width is $L/H = 100$ (see Fig. 1). In the $x$ direction, the inlet ($i = 1$) and outlet ($i = N_x$) pressures are $P_{in}$ and $P_{\text{out}}$, respectively. In the $y$ direction, $j = 1$ and $j = N_y$ represent solid nodes and $j = (2)$: $(N_y - 1)$ are fluid nodes.

## 3. TRT-LBE

In this study, the TRT method, which is proposed by Ginzburg [16], is implemented to study gas flow behavior in a long micro/nano-channel. This model uses two relaxation times, which can be written as:

$$f_i(x + c_i\delta t, t + \delta t) - f_i(x, t) = -\frac{f_i^s - f_i^{seq}}{\tau_s} - \frac{f_i^a - f_i^{aeq}}{\tau_a}, \tag{2}$$

where $f_i$ is the distribution function for a particle at position $x$, $y$ and time $t$ moving with velocity $c_i$. Superscripts $s$ and $a$ indicate the symmetrical and antisymmetrical parts of the distribution function, respectively [17], and $\tau$ is the relaxation time. The symmetrical and antisymmetrical distribution functions and their equilibrium distribution functions can be given as follows:

$$f_i^s = \frac{1}{2}(f_i + f_{-i}), \qquad f_i^{seq} = \frac{1}{2}(f_i^{eq} + f_{-i}^{eq}), \tag{3}$$

$$f_i^a = \frac{1}{2}(f_i - f_{-i}), \qquad f_i^{aeq} = \frac{1}{2}(f_i^{eq} - f_{-i}^{eq}), \tag{4}$$