Thermal Lattice Boltzmann Method for micro-Poiseuille gas flow

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Abstract. In this paper, the thermal Lattice Boltzmann Method (TLBM) is used to simulate a gas microflow. The simulated gas is confined within an inlet/outlet microchannel and driven by a constant inlet velocity $U_{in}$. The bottom wall temperature is taken to be equal zero while the top wall temperature is decreasing from 1 to 0. For consistent results velocity slip and temperature jump boundary conditions at the walls are used. The rarefaction effects given by the Knudsen number, on the velocity and temperature profile are investigated. The results obtained from the TLBM are compared with those obtained using the Finite Difference Method (FDM). In addition to the good agreement observed between the two methods, the results show an interesting sensitivity of velocity and temperature profiles with the gas rarefaction degree.

1. Introduction

During the past few years, the Micro/Nanoelectro-mechanical systems (MEMS/NEMS) [1] technology has known a significant development. Many researchers have investigated the applicability of LBM in these micro and Nano-devices which are used in various fields, such as medicine, electronic, and environment control, etc.

The validity of such approach for describing a gas behavior is mainly related to the flow rarefaction degree according to the Knudsen number value. The gas flow regimes can be classified as follows:

- For $Kn < 0.001$, the continuum regime;
- For $0.001 < Kn \lesssim 0.1$, the slip regime;
- For $0.1 < Kn \lesssim 10$, the transition regime;
- For $Kn > 10$, the gas can be considered in the free molecular regime.

In the literature, very few numerical studies traits the rarefied gas microflows using LBM. Nie et al. [2] applied the LBM method in the transitional regime for compressible flow in microchannels and micro-cavities. In their study, using the bounce-back boundary condition, they have demonstrated that the LBM can capture the fundamental behavior of flows in microchannel flows, including velocity slip, nonlinear pressure drop along the channel and mass flow rate variation with Knudsen number.

Tang et al. [3] defined a reflection coefficient $r_f$, which $r_f = 1$ corresponds to the pure bounce reflection, while, $r_f = 0$ is for a pure specular reflection and it can be taken between 0 and 1 to combine both of boundary conditions.
Zou and He [4] proposed a new method to specify boundary conditions in the consistency with the wall boundary condition, based on the idea of bounce-back of the non-equilibrium distribution function. When these conditions are used together with the incompressible LBGK model, the simulation results recover the analytical solution of the planer Poiseuille flow driven by a pressure gradient. The half-way wall bounce back boundary condition is also used with the pressure density inlet/outlet conditions proposed in this paper to study 2D Poiseuille flow and 3D square duct flow. The numerical results accuracy is approximately of second-order.

Tang et al. [5] proposed a thermal boundary condition for a double-population thermal lattice Boltzmann equation (TLBE) in order to solve two-dimensional Poiseuille and Couette flow. The results agree well with (FVM) and analytical solutions.

Gokaltun and Dulikravich [6] have simulated thermal micro-Couette and thermal micro-Poiseuille by using inlet/outlet boundary conditions to generate a forced convection problem. The calculation of equilibrium distributions at the wall surfaces is modified to incorporate the velocity slip and temperature jump conditions. The effect of the Knudsen number on the velocity and temperature profile is investigated.

Yasuoka et al. [7] applied a mixture of the diffuse scattering and constant wall temperature conditions to obtain thermal jump at the walls. The proposed set of schemes is validated by reference data for Fourier flow and the one around a square cylinder confined in a microchannel.

Zhang and Sun [8] have used the Chapman-Enskog expansion, to prove the consistency of the LBM method with macroscopic conservation laws. They simulated Rayleigh-Benard heat convection problem. The results are interesting and reasonable and meet the experimental data well. The stability of this scheme is also proved through different cases with a large range of Rayleigh number.

Perumal et al. [9, 10] have used diffuse scattering boundary conditions and a combination of bounce-back and specular reflection to capture the slip velocity at the walls in the cases of micro-Couette, micro lid-driven cavity, and micro-Poiseuille flows.

Recently, Zarita and Hachemi [11, 12] have simulated fluid flow and heat transfer inside microchannel, slip velocity and temperature jump boundary conditions are used for the microchannel simulations with Knudsen number values covering the slip regime.

In the present study, the TLBM is used to simulate micro-Poiseuille flow for both cases of isothermal and non-isothermal channel walls temperature. The variation of slip velocity and temperature jump obtained with the current TLBM is compared with the prediction of FDM approach in the slip regime.

2. Problem statement

Two cases of micro-Poiseuille flow are treated, in the first case the temperature of the upper and lower plates is $T_C$, however, the temperature of the upper plate is decreasing from $T_H$ to $T_C$ as a function of $x$-coordinate in the second case as follows:

$$ T(x) = T_H - \left(\frac{T_H - T_C}{L}\right)x. \quad (1) $$

Fig 1. Domain configuration.

3. Numerical method

3.1. Thermal Lattice Boltzmann Method

A square grid and D2Q9 model is used for both distribution functions of density $f$ and temperature $g$. The governing equations for these distribution functions are written according to the Bhatnagar-Gross-Krook (BGK) [13] model as:
\[f_k(x + c_k\Delta t, t + \Delta t) = f_k(x, t) \left( 1 - \frac{1}{\tau_f} \right) + \frac{1}{\tau_f} f_k^{eq}(x, t),\] (2a)

\[g_k(x + c_k\Delta t, t + \Delta t) = g_k(x, t) \left( 1 - \frac{1}{\tau_g} \right) + \frac{1}{\tau_g} g_k^{eq}(x, t).\] (2b)

In which \(\tau_f\) and \(\tau_g\) represent the relaxation times of density and internal energy functions, respectively. The corresponding kinematic viscosity \(\nu\) and thermal diffusivity \(\alpha\) are respectively:

\[\nu = (\tau_f - 1/2)c_s^2\Delta t, \quad \alpha = (\tau_g - 1/2)c_s^2\Delta t.\]

In lattice: \(c_s = c/\sqrt{3} = \sqrt{RT}\).

Where \(c_s\) the velocity of sound, \(R\) is the gas constant and \(T\) is the gas temperature.

The coefficients of viscosity \(\nu\) and thermal diffusion \(\alpha\) are related to the Prandtl number \(Pr\) by \(Pr = \nu/\alpha\).

At the equilibrium state, the Maxwell distribution functions \(f_k^{eq}\) and \(g_k^{eq}\) are written in the Taylor expansion as:

\[f_k^{eq}(k, i, j) = w_k\rho(i, j) \left[ 1 + 3 \frac{c_k u}{c_s^2} + \frac{9}{2} \frac{(c_k u)^2}{c_s^4} - \frac{3}{2} \frac{u^2}{c_s^2} \right],\] (3a)

\[g_k^{eq}(k, i, j) = w_k T(i, j) \left[ 1 + 3 \frac{c_k u}{c_s^2} + \frac{9}{2} \frac{(c_k u)^2}{c_s^4} - \frac{3}{2} \frac{u^2}{c_s^2} \right].\] (3b)

Where the weight factors \(w_k\) are \(w_0 = 4/9, w_{1-4} = 1/9\), and \(w_{5-8} = 1/36\). The discrete scheme D2Q9 is characterized by:

\[c_k = \begin{cases} (0, 0), & k = 0 \\ c \left( \cos \left( \frac{(k-1)\pi}{2} \right), \sin \left( \frac{(k-1)\pi}{2} \right) \right), & k = 1-4 \\ c \left( \cos \left( \frac{(k-5)\pi}{4} \right), \sin \left( \frac{(k-5)\pi}{4} \right) \right), & k = 5-8 \end{cases} \] (4)

The macroscopic density \(\rho\), velocity \(u\) and internal energy by unit of mass \(e\), are obtained by the following relations:

\[\rho = \sum_{k=0}^{9} f_k,\] (5a)

\[\rho u = \sum_{f=0}^{9} c_k f_k,\] (5b)

\[\rho e = \sum_{f=0}^{9} g_k.\] (5c)

Where \(e = DRT/2\), in which \(D\) is the number of physical dimensions (equal to 2 in the current work).

### 3.2. Flow and temperature boundary conditions

In this study, the boundary conditions proposed by Zou and He [4] are used at the inlet and a simple extrapolation scheme is used for velocity at the outlet.

Slip boundary condition are used at the top and bottom walls [14]. At the bottom wall the unknown distributions functions \((f_2, f_5, f_6)\) are calculated as follows:

\[u_{x, y=0} = \lambda \left( \frac{4u_{x, y=0}}{2+3} \right),\] (6a)

\[\rho_{\text{bot}} = f_0 + f_3 + 2(f_4 + f_7 + f_8),\] (6b)

\[f_2 = f_4,\] (6c)

\[f_5 = \frac{\rho_{\text{bot}}(1+u_{x, y=0}) - (f_0 + f_2 + f_6)}{2} - (f_1 + f_8),\] (6d)

\[f_6 = \frac{\rho_{\text{bot}}(1-u_{x, y=0}) - (f_0 + f_2 + f_6)}{2} - (f_3 + f_7).\] (6e)

Where the gas mean free path is defined as \(\lambda = Kn H\), \(Kn\) is the Knudsen number and \(H\) is the total number of lattice nodes in the vertical direction. Temperature jump boundary condition is written at the bottom wall as [14]:

\[T_{y=0} = \frac{C_{\text{jump}}(4T_1 - 2T_2 + 2T_{\text{wall}})}{2+3C_{\text{jump}}}.\] (7)

\(C_{\text{jump}}\) is the temperature jump coefficient defined as:

\[C_{\text{jump}} = \phi \left( \frac{2Y}{(1+Y)Pr} \right) \lambda = k \lambda.\] (8)

In which \(\phi\) represents the thermal-accommodation coefficient and is assumed to be unity, \(Y\) is the specific heat ratio.
3.3. Nusselt number calculation

The heat transfer characteristic of the flow can be determined using the Nusselt number calculated on the bottom wall as follows:

\[ Nu(x) = \frac{2 t \frac{\partial T}{\partial y}}{T_{\text{wall}} - T_{\text{bulk}}} \]  \hspace{1cm} (9)

3.4. Finite Difference Method

The advection-diffusion equation in 2D can be expressed by

\[ T^{n+1}(i,j) = \frac{1}{\tau_g} \left( T^n(i+1,j)+T^n(i-1,j)+T^n(i,j+1)+T^n(i,j-1) \right) + T^n(i,j) \left( 1 - \frac{1}{\tau_g} \right) - u \Delta t \left( \frac{T^n(i,j)-T^n(i-1,j)}{\Delta x} \right) \]  \hspace{1cm} (10)

Where \( n \) is the number of the time step \( \Delta t \), and \( \frac{1}{\tau_g} = \frac{2 u \Delta t}{\Delta x^2} \).

Temperature jump boundary conditions used in TLBM approach are also used in FDM approach at the bottom and the top walls and the following theoretical velocity profile across a microchannel used in the FDM method is:

\[ u(y) = \frac{6 u_{\text{mean}} (\frac{y}{H})^{2+2Kn} \Delta y}{(1+6 \frac{y}{H}^{2+2Kn})} \]  \hspace{1cm} (11)

Where \( \sigma \) is the momentum-accommodation coefficient which is assumed to be equal unity, for full diffuse reflection [15].

4. Results and discussion

In order to validate the method presented in this paper, 2D channel flow between two parallel plates at rest has been simulated. Two cases of micro-Poiseuille flow are treated, in the first case the temperature of the upper and lower plates is \( T_C \), however, the temperature of the upper plate is decreasing from \( T_H \) to \( T_C \) in the second case. To describe easily the results it is more convenient to use the following normalization for temperature: \( \theta = \frac{T-T_C}{T_H-T_C} \), the temperatures \( T_{\text{inlet}} \), \( T_H \), and \( T_C \) become respectively \( \theta_{\text{inlet}} = \theta_H = 1 \), and \( \theta_C = 0 \) [11]. In this study, we take \( Pr = 0.71 \), \( k = 1.667 \) and Reynolds number is fixed at \( Re = 10 \).

4.1. Validation test

To ensure the validation of the method TLBM, the first case is treated and the results are compared with the results presented in Zarita et al. [11] and the FDM approach (see Figs. 2, 3, and 5). To observe the rarefaction effect on the gas flow behavior, the velocity profiles for \( Kn = 0.01 \) and 0.08 (Fig. 2), and the temperature profiles for \( Kn = 0.01 \), 0.05, and 0.08 (Fig. 3) are plotted. Figures show the effect of \( Kn \) on the velocity slip and temperature jump at the centerline of the microchannel. Good agreement between the analytical solution and TLBM approach for horizontal velocity along the centerline vertical axis is observed. It is shown that velocity slip is sensitive to the rarefaction degree near the longitudinal walls. Therefore, the kinetic slip-jump phenomena are well captured by TLBM in the slip regime mainly encountered in MEMS devices. To compare the transient time of both solutions given by FDM and TLBM approaches, the temperature profile is plotted as a function of time steps number for \( Kn = 0.01 \), and 0.1. For a given \( Kn \), the TLBM and FDM require the same time to reach steady state (7000 steps) and with increasing of \( Kn \), the temperature value in the equilibrium state at the bulk increases (Fig. 4). The convergence of the Nusselt number to a constant value is reached as soon as the velocity and the temperature become constant (Fig. 5), and the temperature contours for \( Kn = 0.05 \) are shown in Figs. 6.

4.2. Mesh size independence

Table 1 shows the effect of the mesh on the horizontal velocity, temperature near the inlet \((x/L = 0.05, y/H = 0.5)\), and on the average Nusselt number by using TLBM approach for the channel aspect ratio \( AR = 4 \). To save the computation time, the grid size 200 × 50 is enough to give good agreement data.
Table 1. Effect of the mesh on the velocity, temperature and average Nusselt number for $Kn = 0.05$.

| Mesh   | 180 × 45 | 200 × 50 | 220 × 50 |
|--------|----------|----------|----------|
| $u/U_{in}$ | 1.08     | 1.08     | 1.08     |
| $\theta$   | 0.963    | 0.964    | 0.963    |
| $Nu$   | 5.27     | 5.26     | 5.26     |

Figure 2. Velocity profiles along the centerline vertical axis according to $Kn$.

Figure 3. Temperature profiles at centerline along the vertical axis according to $Kn$.

Figure 4. Evolution of the temperature at the center of the microchannel.

Figure 5. Nusselt number variation along the microchannel according to $Kn$.

Figure 6. Temperature isolines (isotherms) in the microchannel.

(a) TLBM - $Kn = 0.05$.

(b) FDM - $Kn = 0.05$. 
4.3. Numerical results and analysis

By using TLBM approach, both cases give the same velocity profiles since Eq. (5b) is independent of the temperature. Using the slip boundary condition, the so-called velocity slip phenomenon is captured. By increasing the rarefaction degree \((Kn)\), the slip velocity increases (see Figs. 7a, and 7b) and the amplitude of the horizontal velocity at the center of the microchannel decreases at the steady state that reached after approximately 2200 steps (Fig. 8). Fig. 9 shows that by increasing the rarefaction degree \((Kn)\), the temperature curve at the channel center reaches a high value (for \(Kn = 0.1\) \(-\theta = 0.556\)). In the horizontal direction, the temperature decreases quickly near the bottom wall \((y/H = 0.01\) and \(y/H = 0.05\)) and reaches a constant value almost equal zero for \(Kn = 0.01\) but this form becomes inclined and the outlet temperature becomes larger because of the gas rarefaction \((Kn = 0.1)\), good agreement between the analytical solution of FDM and TLBM as shown in figs. 10a, 10b, 11a, and 11b. However, in the vertical direction, the temperature profile loses its parabolic form. The temperature is sensitive to the Knudsen number for both walls, and by increasing the rarefaction degree \(Kn\), the temperature jump increases (see Figs. 11a, 11b, and Table 2). The amplitude of the temperature near the channel inlet \((x/L = 0.01\) and \(x/L = 0.05\)) takes a value almost equal 1 when \(y/H > 0.5\). For both cases, by increasing the value of Knudsen number, the average value of the Nusselt number decreases, but in the second case, this decreasing becomes more pronounced (Table 3, and Fig. 12). The temperature contours for \(Kn = 0.05\) are shown in Figs. 13a, and 13b and it is observed that both approaches give the same temperature isolines. This shows that non-uniform wall temperature affects significantly the thermal transfer in the channel.

The temperature jump is calculated at the center of the top wall as follows:

\[
\theta_{\text{jump}} = \theta \left(\frac{x}{L} = 0.5\right) - \theta_{\text{wall}}. \tag{12}
\]

![Figure 7. Velocity profile along the vertical axis.](image)

(a) \(Kn = 0.01\).

![Figure 8. Evolution of the horizontal velocity at the center of the microchannel.](image)

(b) \(Kn = 0.1\).

![Figure 9. Evolution of the temperature at the center of the microchannel.](image)
Figure 10. Temperature profile along the horizontal axis.

(a) $Kn = 0.01$.  
(b) $Kn = 0.1$.

Figure 11. Temperature profile along the vertical axis.

(a) $Kn = 0.01$.  
(b) $Kn = 0.1$.

Figure 12. Nusselt number variation along the microchannel according to $Kn$.

(a) TLBM - $Kn = 0.05$.  
(b) FDM - $Kn = 0.05$.

Figure 13. Temperature isolines (isotherms) in the microchannel.

(a) TLBM - $Kn = 0.05$.  
(b) FDM - $Kn = 0.05$.  

(a) $Kn = 0.01$.  
(b) $Kn = 0.1$.
Table 2. Effect of $Kn$ on the temperature jump at the center of top wall.

| $Kn$ | TLBM | FDM |
|------|------|-----|
| 0.01 | 0.00401 | 0.00388 |
| 0.1  | 0.05805 | 0.05692 |

Table 3. Value of average Nusselt number at different $Kn$ by TLBM approach.

| $Kn$ | First case | Second case |
|------|------------|-------------|
| 0.01 | 8.34       | 6.43        |
| 0.05 | 6.62       | 5.26        |
| 0.1  | 5.31       | 4.39        |

5. CONCLUSION

The TLBM with slip and jump boundary conditions is used to simulate the gas flows in microchannel with isothermal and non-isothermal walls. It is observed that non-isothermal wall has a significant effect on both thermal and hydrodynamic flow behaviors. The slip-jump boundary conditions allow capturing of non-equilibrium effect near the walls. Good agreement is observed between the approaches TLBM and FDM. So, regarding its fast convergence, the TLBM is, therefore, a good alternative that can be used to describe the gas microflows usually encountered in the MEMS/NEMS devices. Unlike the pure kinetic methods, like the direct simulation of Monte Carlo (DSMC), which needs a long time to achieve satisfactory results.

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