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An improved thermal lattice Boltzmann model for rarefied gas flows in wide range of Knudsen number ☆

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ABSTRACT

In order to covering a wide range of the flow regimes, a new relaxation time formulation for the lattice Boltzmann method, LBM, by considering the rarefaction effect on the viscosity and thermal conductivity has been presented. To validate the presented model, fully developed pressure driven flow and developing thermal flow in micro/nano channel have been modeled. The results show that in spite of the standard LBM, the velocity and temperature distributions, the volumetric flow rate and the local Nusselt number obtained from this modified thermal LBM, agree well with the other numerical and empirical results in a wide range of Knudsen numbers.

1. Introduction

By reducing the dimensions of a channel, heat transfer area per unit volume increases and therefore the overall heat transfer coefficient per unit volume increases. Flow and heat transfer in micro/nano devices is different from macro devices. This is because of the fact that when the mean free path, λ, of the molecules becomes comparable to the characteristic length of the flow domain, the continuum flow model (Navier Stokes equations) breaks down and the Knudsen number, Kn, defined as the ratio of the molecular mean free path to the characteristic length of the system, increases. For $Kn<10^{-3}$ the continuity assumption with no slip boundary conditions is valid. For $10^{-3}<Kn<10^{-1}$ (slip flow regime) the velocity and temperature of the gas near the wall are no longer equal to the wall velocity and temperature respectively and for $Kn>10^{-1}$ (transition and free molecular flow regime) the continuity assumption is under question [1].

Although molecular based methods such as Molecular Dynamic (MD) simulation and Direct Simulation Monte Carlo (DSMC) methods [2] have made some progresses in micro/nano fluidic flow simulations [3,4], they are often too expensive for most practical applications. A midway approach is the Lattice Boltzmann Method, LBM, obtained by discretization of Boltzmann equation in time and velocity space [5]. In principle the Lattice Boltzmann Equation (LBE) is a more fundamental equation compared to the Navier Stokes equations, which is valid for all ranges of Knudsen number [6,7], thus, it has been believed that the LBM has a greater potential to model high Knudsen flows than the methods based on the Navier Stokes equations [8].

Recently there have been attempts to use the LBM for gaseous flows in slip flow regime [9–15] but only a few papers can be mentioned for the use of LBM in transition regime [16–23]. To this end, two methods are proposed based on the use of higher order LBM [16–19] and the modification of the mean free path [18–22]. 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. [18] have demonstrated that the high order LBMs have improved current capability but Kim et al. [19] 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 [24].

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. [22] 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.

All of the mentioned articles investigated the isothermal (athermal) flows. Current thermal LBE models are confined to the continuous and slip flow regimes [25–31] and the use of the LBM for higher Kn regimes has not been successful so far.

In the previous article [23], we proposed a new relaxation time formulation in such a way that wide range of Kn regimes of flow can be simulated more accurately. In this article, by relating the thermal conductivity to the local Kn, a new thermal relaxation time model is suggested which can simulate wide range of thermal flow regimes.

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2. Thermal lattice Boltzmann method

The continuum Boltzmann equation is a fundamental model for rarefied gases in the kinetic theory [32,33]. 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. In this article the two distribution function thermal lattice Boltzmann model based on the work of He et al. [34] is used which utilizes two different distribution functions, one for the velocity field (f) and the other for the internal energy field (g):

$$\partial_t f + \left(\vec{\xi}.\nabla\right) f = \frac{f - f^{\mathrm{eq}}}{\lambda_f} \tag{1}$$

$$\partial_t g + \left(\vec{\xi}.\nabla\right) g = \frac{g - g^{\mathrm{eq}}}{\lambda_g} \tag{2}$$

where λ_f and λ_g are the relaxation times for the number and energy density distribution functions respectively, and f^{eq} and g^{eq} are the equilibrium distribution functions approximated as Maxwellian form given by Eqs. (3), (4):

$$f^{\mathrm{eq}} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{\left(\vec{\xi}-\vec{u}\right)^2}{2RT}\right) \tag{3}$$

$$g^{\mathrm{eq}} = \frac{\rho\left(\vec{\xi}-\vec{u}\right)^2}{2(2\pi RT)^{3/2}} \exp\left(-\frac{\left(\vec{\xi}-\vec{u}\right)^2}{2RT}\right) \tag{4}$$

where R is the gas constant and ρ, $\vec{u}$ and T are density, velocity and temperature, respectively.

In the present work, the nine velocity 2D model (D2Q9), is used to discrete momentum space (Fig. 1) [35]. In this model, the discrete velocity field $\vec{c}_i = (c_{ix}, c_{iy})$ is:

$$\vec{c}_i = \begin{cases} (0,0), & i = 0 \\ \left(\cos\left(\frac{i-1}{2}\pi\right), \sin\left(\frac{i-1}{2}\pi\right)\right)c, & i = 1,\ldots,4 \\ \sqrt{2}\left(\cos\left(\frac{2i-9}{4}\pi\right), \sin\left(\frac{2i-9}{4}\pi\right)\right)c, & i = 5,\ldots,8 \end{cases} \tag{5}$$

where $c = \Delta x/\Delta t$. Δx and Δt are lattice spacing and time step, respectively. He et al. [34] used a second order discretization scheme for Eqs. (1), (2). The resulting equations are:

$$\bar{f}_i(\vec{x} + \vec{c}_i\Delta t, t + \Delta t) - \bar{f}_i(\vec{x}, t) = -\frac{1}{\tau_f + 0.5}\left[\bar{f}_i(\vec{x}, t) - f_i^{eq}(\vec{x}, t)\right] \tag{6}$$

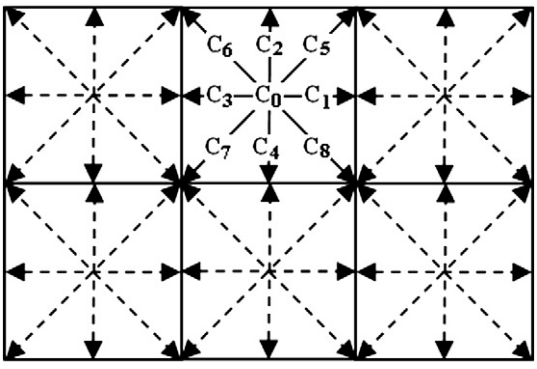

Fig. 1. Configuration of the lattice and discrete velocity vectors, D2Q9 model.

$$\bar{g}_i(\vec{x} + \vec{c}_i\Delta t, t + \Delta t) - \bar{g}_i(\vec{x}, t) = -\frac{1}{\tau_g + 0.5}\left[\bar{g}_i(\vec{x}, t) - g_i^{eq}(\vec{x}, t)\right] \tag{7}$$

where $\tau_f = \lambda_f/\Delta t$ and $\tau_g = \lambda_g/\Delta t$ are the non-dimensional relaxation times. The new variables are introduced in order to have an explicit scheme, i. e.

$$\bar{f} = f + \frac{1}{2\tau_f}(f - f^{eq}) \tag{8}$$

$$\bar{g} = g + \frac{1}{2\tau_g}(g - g^{eq}) \tag{9}$$

The functions f^{eq} and g^{eq} can be calculated through a second order Taylor series expansion of the Maxwell distribution function, Eqs. (3), (4), followed by a discretization of the result on the D2Q9 lattice, which results in:

$$f_i^{eq}(\vec{x}, t) = \rho.w_i\left(1 + \frac{\vec{u}.\vec{c}_i}{RT} + \frac{(\vec{u}.\vec{c}_i)^2}{2(RT)^2} - \frac{\vec{u}.\vec{u}}{2RT}\right)$$
$$w_0 = \frac{4}{9}, w_{i=1,2,3,4} = \frac{1}{9}, w_{i=5,6,7,8} = \frac{1}{36} \tag{10}$$

$$g_i^{eq}(\vec{x}, t) = \begin{cases} -w_0\rho\varepsilon\frac{3(\vec{u}.\vec{u})}{2c^2} & i = 0 \\ g_\alpha^{eq} = w_0\rho\varepsilon\left[1.5 + \frac{1.5\vec{c}_i.\vec{u}}{c^2} + \frac{4.5(\vec{c}_i.\vec{u})^2}{c^4} - \frac{1.5(\vec{u}.\vec{u})}{c^2}\right] & i = 1,2,3,4 \\ g_\alpha^{eq} = w_0\rho\varepsilon\left[3 + \frac{6\vec{c}_i.\vec{u}}{c^2} + \frac{4.5(\vec{c}_i.\vec{u})^2}{c^4} - \frac{1.5(\vec{u}.\vec{u})}{c^2}\right] & i = 5,6,7,8 \end{cases} \tag{11}$$

The flow parameters are then calculated in terms of the particle distribution function $f_i(\vec{x}, t)$, by:

$$\rho = \sum_i \bar{f}_i, \quad \rho\vec{u} = \sum_i c_i\bar{f}_i, \quad \rho\varepsilon = \rho RT = \sum_i \bar{g}_i \quad \upsilon = c_s^2\tau_f \tag{12}$$

3. LBM for high Knudsen number flows

From the DSMC method and the linearized Boltzmann equation [36], it is evident that the velocity profiles of flow in a channel in the transition and free molecular regimes remain approximately parabolic. But the velocity profile obtained from continuum based relations does not predict the flow rate properly. This is because of the fact that the dynamic viscosity which is related to the diffusion of momentum due to the intermolecular collisions must be modified to consider the diffusion of momentum due to the intermolecular collisions and the collision of molecules with the walls. The kinetic theory description for dynamic viscosity requires:

$$\mu_0 = \lambda\bar{v}\rho \tag{13}$$

where $\bar{v}$ is the mean thermal speed. Using the mean free path, λ, in this relation is valid as long as intermolecular collisions are dominant (e. g. $\mathrm{Kn} \ll 1$). However, for increased rarefaction the intermolecular collisions are reduced significantly and in the free molecular flow regime only the collisions of the molecules with the walls should be considered. Therefore Polard and Present [37] suggested that for the free molecular channel flow the dynamic viscosity should be based on the characteristic length scale, h;

$$\mu_\infty = h\bar{v}\rho \tag{14}$$

Since the diffusion coefficient is based on λ in slip or continuum flow regimes and *h* in the free molecular flow regime, Karniadakis and Beskok [1] considered an effective dynamic viscosity to model the variation of diffusion coefficient:

$$\mu_{\text{eff}} = \rho\bar{v}\left[\frac{1}{\frac{1}{\lambda}+\alpha\frac{1}{h}}\right] = \frac{\mu_0}{1+\alpha Kn} \tag{15}$$

The value $\alpha = 2.2$ was suggested in their effort to match their numerical results for the mass flow rate in a channel with the corresponding DSMC results.

The thermal conductivity, *k*, of a gas is a function of its density as well as its temperature. Specifically, *k* is proportional to the mean free path with the proportionality coefficient a general function of temperature, i.e. [1],

$$k_0 = F\left(\frac{T}{T_0}\right)\rho\sqrt{2RT}R\lambda \tag{16}$$

Similar to the dynamic viscosity, the characteristic length scale of the thermal conductivity in the free molecular channel flow is the channel dimension, *h*:

$$k_\infty = F\left(\frac{T}{T_0}\right)\rho\sqrt{2RT}Rh \tag{17}$$

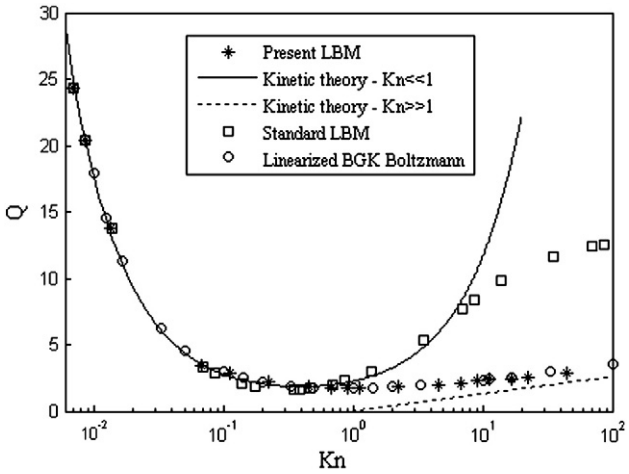

Fig. 3. Volumetric flowrate as a function of exit Kn.

Thus, we have proposed the following hybrid formula to model the variation of thermal conductivity:

$$k_{eff} = F\left(\frac{T}{T_0}\right)\rho\sqrt{2RT}R\left[\frac{1}{\frac{1}{\lambda}+\alpha\frac{1}{h}}\right] = \frac{k_0}{1+\alpha Kn} \tag{18}$$

From the kinetic theory, the kinematic viscosity is $\upsilon = 1/2\bar{c}\lambda$ where $\bar{c} = \sqrt{8RT/\pi}$ is the mean molecular velocity. Combined with

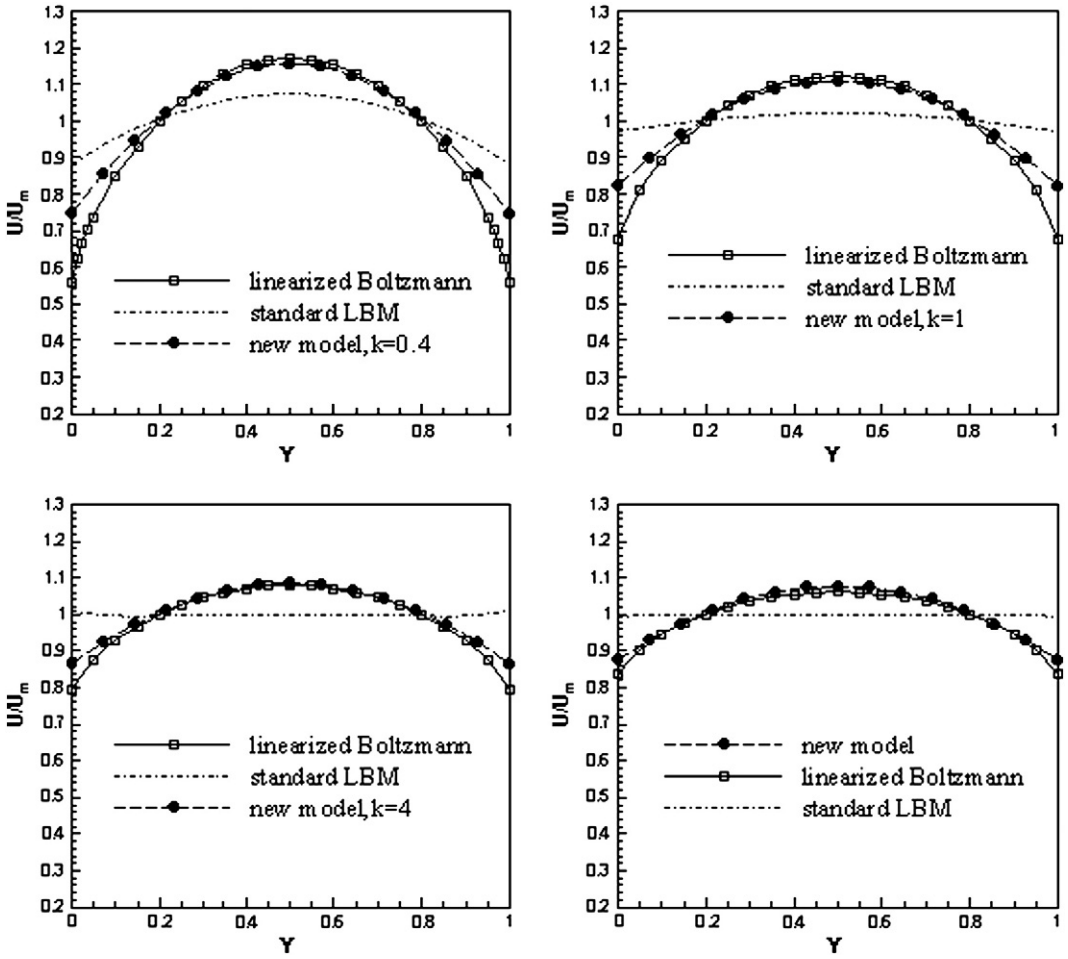

Fig. 2. Normalized velocity distribution across the micro/nano channel.

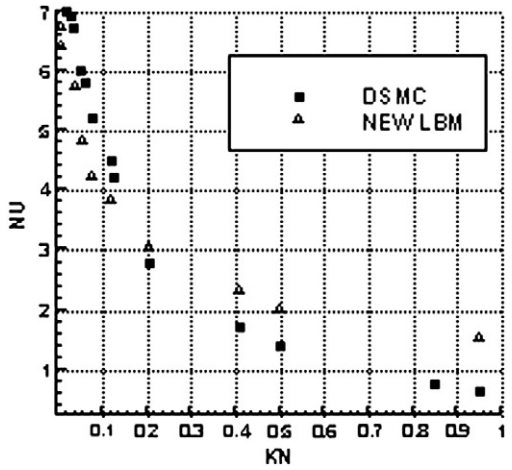

Fig. 4. Nusselt number obtained from the DSMC and the new LBM.

the kinematic viscosity expression of LBM ($\upsilon = c_s^2 \tau_f$) and by using the effective viscosity, we have defined a new effective relaxation time in the LBM as follows:

$$\tau_{eff} = \frac{Kn}{1 + \alpha Kn} N \tag{19}$$

where N is the number of lattice across the characteristic length of the flow domain. The thermal relaxation time can be obtained from the following relation:

$$\tau_g = Pr\,\tau_{eff} \tag{20}$$

Therefore, modifying the hydrodynamic relaxation time, τ_f, modifies the thermal relaxation time spontaneously.

4. Results and discussion

4.1. Fully developed pressure driven flow

In order to validate the presented model, pressure driven flow in micro/nano channel with different Knudsen numbers, are simulated. The slip reflection boundary condition (SRBC) [38] which is a combination of the bounce back and specular boundary conditions is used to predict the slip velocity on solid walls. In Fig. 2 the non-dimensional velocity profiles normalized by local average velocity which is obtained in the transition flow regime for $K = 0.1$ to 10 is plotted across the channel, where K is $(\sqrt{\pi}/2)Kn$. The corresponding linearized Boltzmann solution is also included [36]. It is seen that the LBM velocity profile and the linearized Boltzmann solution agree quiet well through the Knudsen numbers up to 10. However, a little discrepancy appears very close to the walls. It is because of the fact that the intermolecular forces between fluid molecules and solid walls become important near the walls, in the transition regime [39].

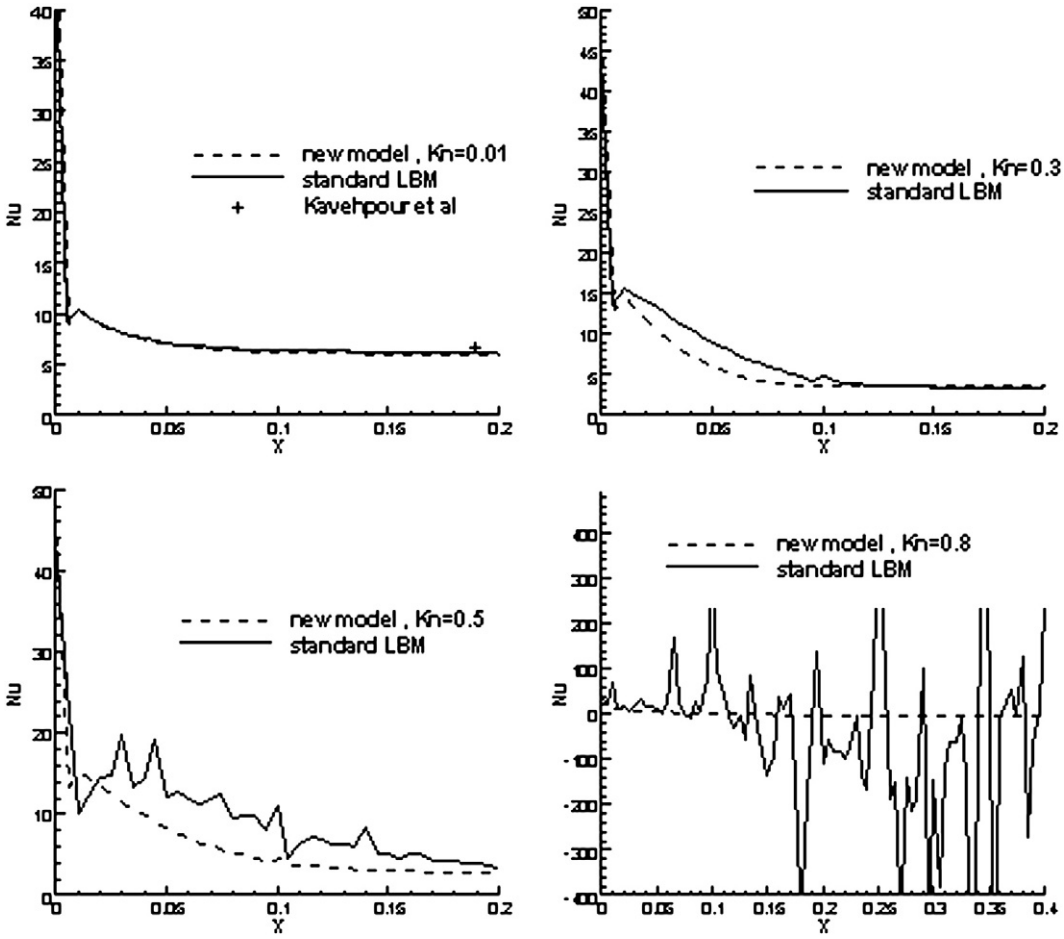

Fig. 5. The Nu values obtained from the standard LBM and modified LBM for different inlet Knudsen numbers.

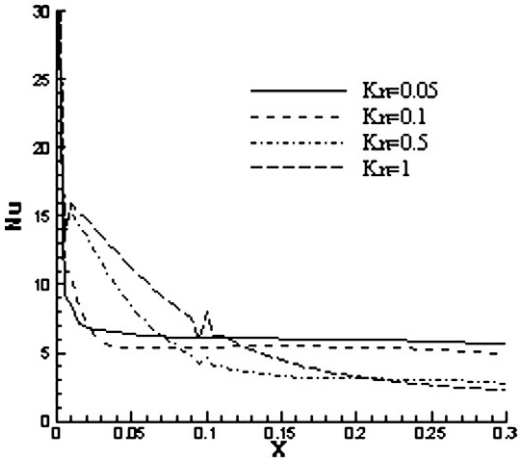

Fig. 6. Local wall Nu for different Kn_{in}.

Fig. 3 shows the normalized flow rate through micro/nano channel as a function of the Knudsen number. It can be seen that by increasing the Knudsen number, the flow rate decreases initially and has a minimum value for $Kn \approx 1$, then it increases [40,7]. This phenomenon is called Knudsen minimum effect [41]. Although from the kinetic theory of gases, there is no analytical formula for flow rate in the transition regime, there are two asymptotes for normalized flow rate which is evident in Eq. (21) [33].

$$\begin{aligned} Q_0 &= (6Kn)^{-1} + s + \left(2s^2 - 1\right)Kn \quad && Kn < 1 \\ Q_\infty &= (1/\sqrt{\pi})\ \ln(Kn) && Kn \to \infty \end{aligned} \tag{21}$$

where $s = 1.015$.

It can be seen from the figure that our results are in good agreement with those of the Eq. (21) as well as the linearized Boltzmann method [7]. In Fig. 3, the results of the standard LBM, are also presented. These results agree very well for flows with Kn less than 0.1, which corresponds approximately to the slip flow regime, but the predicted flow rate is overestimated in the early transition flow regime for Kn > 0.4 and diverges from results of linearized Boltzmann method [42,43]. However, the present results by modifying LBM are accurately compatible with linearized Boltzmann method in the entire transition flow regime. As shown in Fig. 3, the Knudsen minimum effect is captured for $Kn \approx 1$ by using our new model.

4.2. Developing thermal flow

The developing thermal flow in micro/nano channels is another test case for the present lattice Boltzmann model. A uniform inlet flow with the velocity $U_0 = 0.1$ and temperature T_0 is imposed at the inlet of the channel. It is assumed that the channel walls are heated uniformly with a constant temperature T_w ($T_w = 10T_0$). In this work,

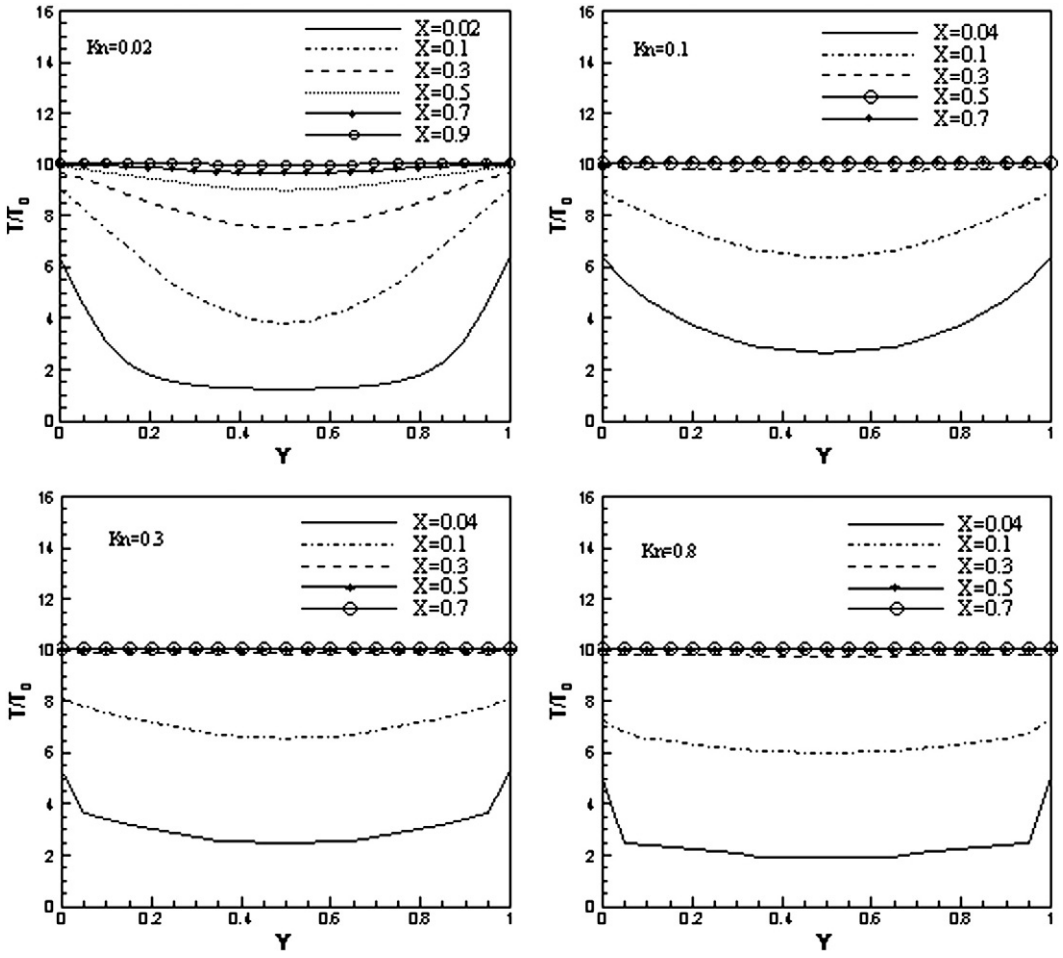

Fig. 7. The temperature distribution at different positions for different inlet Knudsen numbers.

the Diffuse Scattering Boundary Condition (DSBC) [44,45] was used for slip velocity and temperature jump boundary conditions.

Fig. 4 compares the values of Nusselt number, Nu, at the fully developed region obtained from the modified LBM with the results based on the DSMC method [46]. During the simulation, the Prandtl number is fixed as Pr = 2/3 and the Nu is defined as

$$\mathrm{Nu} = \frac{2H(\partial T/\partial y)_{\mathrm{w}}}{(T_{\mathrm{w}} - T_B)} \tag{15}$$

where T_B is the bulk temperature and H is the channel width. It can be seen from the figure that the results, have good agreement for $Kn \leq 0.2$ but by increasing the Knudsen number, the LBM over predicts the Nu values, but it can be seen from Fig. 5 that the Nu values obtained from the modified LBM are less than those of the standard LBM. Therefore the new model modifies the results of LBM.

Fig. 5 shows the Nu values obtained from the standard LBM and modified LBM along the entrance region of the channel for $Kn_{in} = 0.01$, 0.3, 0.5, and 0.8. In the present work Pr is fixed as 0.7 but, Kn is variable along the channel and can be expressed as [47]:

$$\frac{\mathrm{Kn}}{\mathrm{Kn}_{in}} = \frac{\bar{u}^*}{\sqrt{T_{\mathrm{B}}^*}} \tag{16}$$

where $\bar{u}^* = \bar{u}/U_0$ and $T_B^* = T_B/T_0$ are non-dimensional average velocity and non-dimensional bulk temperature respectively. Furthermore, the steady state Nu obtained from the numerical solutions based on the compressible momentum and energy equations with slip velocity and temperature jump boundary conditions is considered for $Kn_{in} = 0.01$[47]. Similar to the high Knudsen numbers (Fig. 4), it can be seen from the figure that for the low values of Kn ($Kn = 0.01$-slip regime) both of the LBMs have the same results, but for $Kn > 0.7$, the standard LBM are completely unstable and cannot present proper results.

Local wall Nu of the thermal developing flows for different Kn_{in} (slip and transitional regimes) is shown in Fig. 6. From the definition of Nu, it can be seen that Nu is inversely proportional to the temperature jump. By increasing Kn, the slip velocity and temperature jump near the wall increases. Therefore, it can be seen from the figure that the increase of Knudsen number causes the fully developed Nusselt number decreased and the entrance region occurs at higher values of X.

In Fig. 7 the temperature distribution along the channel is shown. From the figure, obvious temperature jumps on the plates can be observed due to the rarefaction effect. As expected, the flow of this kind quickly becomes fully developed after a short entrance region where the hydrodynamic and thermal boundary layers are simultaneously developed.

5. Conclusion

The new LBM is capable of simulating the flow and heat transfer for a wide range of Knudsen numbers including the transition regime. It is shown that the proposed model by modifying the relaxation time in LBM is able to predict the flow features in micro and nano scales for wide range of Kn, accurately. Non-dimensional velocity distribution and the well-known Knudsen minimum effect in micro and nano channels are achieved for $Kn \approx 1$ and local Nusselt numbers are in good agreement with the exiting numerical data for $Kn \leq 0.2$.

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