Provide a suitable range to include the thermal creeping effect on slip velocity and temperature jump of an air flow in a nanochannel by lattice Boltzmann method

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ABSTRACT
The thermal creeping effect on slip velocity of air forced convection through a nanochannel is studied for the first time by using a lattice Boltzmann method. The nanochannel side walls are kept hot while the cold inlet air streams along them. The computations are presented for the wide range of Reynolds number, Knudsen number and Eckert number while slip velocity and temperature jump effects are involved. Moreover appropriate validations are performed versus previous works concerned the micro–nanoflows.

The achieved results are shown as the velocity and temperature profiles at different cross sections, streamlines and isotherms and also the values of slip velocity and temperature jump along the nanochannel walls. The ability of the lattice Boltzmann method to simulate the thermal creeping effects on hydrodynamic and thermal domains of flow is shown at this study; so that its effects should be involved at lower values of Eckert number and higher values of Reynolds number especially at entrance region where the most temperature gradient exists.

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1. Introduction

Micro and NanoElectro Mechanical Systems (MEMS and NEMS) are considered as the one of main favorite research topics nowadays. Flow properties in microscale regimes are different from the macro ones; so that well known Knudsen number \((Kn=\lambda/D_H)\) is used to classify the micro–nanoflows where \(\lambda\) represents the molecular mean free path. The fluid flow is supposed as continuum at \(Kn<0.001\) and Navier–Stokes equations could be used to simulate the flow field at this state [1–5]. However other regimes as like the slip flow, transient and free molecular can be achieved at \(0.001<Kn<0.1\), \(0.1<Kn<10\) and \(Kn>10\), respectively [6–11].

Navier–Stokes methods with slip velocity boundary condition beside the particle based methods are able to investigate the slip flow regime. The trace and collision between the molecular and particles of a gas flow are the main objects of particle based methods including lattice Boltzmann method (LBM), direct simulation of Monte Carlo (DSMC) and molecular dynamics (MD) [12–16]. Among them, LBM shows less cost of computation and also works with simpler math equations than MD or DSMC which makes LBM more functional for the microflows [17–22].

LBM consists of collision and propagation between the particles placed on the specified locations on a lattice. In this approach, the fluid domain is considered by the fictive particles which each one has been made of too many molecular. LBM is almost a new model which deals better with the complex boundaries than the CFD methods. Moreover LBM uses the simple and parallel algorithm that can be used for a wide range of Knudsen number [23–28]. However it should be mentioned that LBM needed an appropriate collision operation to avoid divergence; in this way, the model of LBM-BGK was developed which showed suitable accuracy and stability [29–31].

Different models of thermal LBM can be referred for the thermal domains. The internal energy distribution function one is able to consider the pressure work and viscous heat dissipation beside its higher numerical stability. This approach is called thermal lattice Boltzmann method (TLBM) which the both of hydrodynamic \((f)\) and thermal \((g)\) distribution functions are used in together [32–38].

Provide a suitable formulation for the boundary conditions in terms of distribution functions is one of disadvantages of LBM so that several researchers are trying to develop the useful practical LBM-boundary conditions. Diffuse scattering boundary condition (DSBC) introduced by Niu et al. [39,40] and Shu et al. [41] represents the relaxation time according to the Knudsen number to determine the slip velocity.
2. Problem statement

Forced convection of air (Pr≈ν/μ=0.7) through a two dimensional nanochannel is studied numerically by using the lattice Boltzmann method (Fig. 1). TLBM-BGK model based on momentum (f) and internal energy (g) distribution functions is chosen to simulate the flow and heat transfer at 0.001≤Kn≤0.1; which implies the slip flow regime at Reynolds number equals to Re=ρuiDh/μ=10,100,1000. The appropriate hydrodynamic and thermal boundary conditions are used in terms of distribution functions needed for LBM. The two dimensional-9 point lattice as D2Q9 is selected which is shown in Fig. 2 [18]. Nanochannel side walls are kept hot at TH while the cold inlet air at TC streams along them. The nanochannel aspect ratio is supposed as AR=L/H=30. The width of channel is considered as H=250 nm which means the length equals to L=7.5 μm. Moreover the mean free path of the air molecules (λ) is almost equals to 50 nm. These facts imply why the authors called the expression of nanochannel to the supposed channel configuration at Kn=0.1. However the phrase of microchannel has been also used in the several previous works.

Present work aims to investigate the effect of thermal creeping on the flow and heat transfer of a nanoflow which has been ignored in the previous works. Moreover the effects of this phenomenon on slip velocity and temperature jump are studied. To do this, the wide range of Eckert number is selected at each section as 0.1<Ec=Ma^2(k−1)τo/ΔT<10.

3. Numerical procedure

3.1. Lattice Boltzmann method

Using density-momentum distribution function, the Boltzmann equation is observed as [33]:

\[ \partial_t f + \mathbf{c} \cdot \nabla f = \Omega(f) \]

(1)

\[ \Omega = 0.5 \left( \mathbf{c} - \mathbf{u} \right)^T f \]

(2)

Greek symbols

\[ \lambda \] molecular mean free path
\[ \nu \] kinematic viscosity (m^2/s)
\[ \theta = (T - T_c)/(T_H - T_c) \] dimensionless temperature
\[ \theta_{f}, \theta_{g} \] dimensionless temperature jump
\[ \rho \] density (kg m^{-3})
\[ \mu \] dynamic viscosity (Pa s)
\[ \tau_f, \tau_g \] momentum and internal energy relaxation times

Super- and sub-scripts

\[ C \] cold
\[ \epsilon \] equilibrium
\[ H \] hot
\[ i \] the link number of lattice, Inlet flow
\[ w \] wall

The schematic figure of the nanochannel.

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which leads to generate the thermal lattice Boltzmann equation according to the internal energy:

\[ \partial_t g + (c \cdot \nabla) g = \mathcal{L}(g) \]

Now the collision operations of LBM-BGK model for hydrodynamic and thermal fields are defined:

\[ \mathcal{L}(f) = - \frac{f - f^e}{\tau_f} \]

\[ \mathcal{L}(g) = - \frac{g - g^e}{\tau_g} - fZ = 0.5(c \cdot \nabla) \mathcal{L}(f) - fZ \]

in which the heat dissipation term \((fZ)\) can be determined as:

\[ fZ = f(c - u) \left[ \partial u + (c \cdot \nabla) u \right] \]

\(\tau_f\) is the hydrodynamic relaxation time and also \(\tau_g\) is the thermal relaxation time, respectively. Now the two new modified functions \(\tilde{f}_i\) and \(\tilde{g}_i\) are presented to avoid from implicitness in Eqs. (1)-(5):

\[ \tilde{f}_i = f_i + \frac{dt}{2\tau_f} (f_i - f^e) \]

\[ \tilde{g}_i = g_i + \frac{dt}{2\tau_g} (g_i - g^e) + \frac{dt}{2} fZ_i \]

The hydrodynamic and thermal Maxwell equilibrium distribution functions are shown as \(f^e_i\) and \(g^e_i\), respectively. It is worth noting that \(\tau^*\) demonstrates the lattice link number; hence \(Z_i\) can be written as follows:

\[ Z_i = (c_i - u). D_j u \text{ and } D_i = \partial_i + c_i \cdot \nabla \]

\[ c_i = \begin{cases} \cos \left( \frac{i - 1}{2} \pi \right), \sin \left( \frac{i - 1}{2} \pi \right) \end{cases} \text{, } i = 1, 2, 3, 4 \]

\[ c_i = \sqrt{2} \left\{ \begin{cases} \cos \left( \frac{(i - 5)}{2} \pi + \frac{\pi}{4} \right), \sin \left( \frac{(i - 5)}{2} \pi + \frac{\pi}{4} \right) \end{cases} \text{, } i = 5, 6, 7, 8 \] \text{ and } c_0 = (0, 0) \]

where the discrete microscopic velocity is stated by \(c_i\). Now the collision and propagation steps are performed by using \(f^e_i\) and \(g^e_i\):

\[ \tilde{f}(x + c_i dt, t + dt) - \tilde{f}(x, t) = - \frac{dt}{\tau_f + 0.5dt} \left[ \tilde{f}_i - f^e_i \right] \]

\[ \tilde{g}(x + c_i dt, t + dt) - \tilde{g}(x, t) = - \frac{dt}{\tau_g + 0.5dt} \left[ \tilde{g}_i - g^e_i \right] - \frac{dt}{2\tau_g} fZ_i \]

For \(D_2 Q_9\) model \(c^2 = 3RT = 1\) and the weight functions are chosen as \(\alpha_{10} = 4/9\) and \(\alpha_{11} = 1/9\), \(i = 1, 2, 3, 4\) and \(i = 1/3, 5, 6, 7, 8\). As a result the macroscopic parameters can be determined as below, while \(\rho_e = \rho R T:\)

\[ \rho = \sum_i \rho_u u_i = \sum_i \frac{c_i}{2} \rho u e = \sum_i \frac{\partial_i}{2} \sum_i f_i Z_i \]

Based on gases kinetic theory, Knudsen number is achieved as follows:

\[ Kn = \sqrt{\frac{2}{\pi}} \frac{Ma}{Re} \]

\(k\) is the heat capacity ratio of a gas. The amounts of relaxation times can be determined according to the definition of variables like \(Re, Ma = u_i/c_i, \tau = \mu/P, P = \rho c^2\) and \(c_i = 1/30.5:\)

\[ \tau_f = \frac{6}{\sqrt{\pi}} \frac{D_{ij}}{\nu} \]

\[ \tau_g = \frac{\tau_f}{Pr} \]

3.2. Boundary conditions

The non-equilibrium bounce back model is applied at the inlet and outlet for the flow field [28,38]:

\[ \tilde{f}_i = f_i + \frac{1}{2} \rho u_i u_i = f_i + \frac{1}{2} (f_i - f^e_i) + \frac{1}{6} \rho u_i u_i f^e \]

\[ \tilde{f}_i = f_i - \frac{1}{2} (f_i - f^e_i) + \frac{1}{6} \rho u_i u_i \]

\[ \tilde{f}_i = f_i + \frac{1}{2} (f_i - f^e_i) - \frac{1}{6} \rho u_i u_i + \frac{1}{2} \rho u_i u_i f^e \]

By using Eqs. (21) and (22) for the thermal boundary conditions at inlet and outlet, the unknown distribution functions at these sections can be calculated, respectively [23]:

\[ \tilde{g}_5 = \frac{6 \rho e + 3d \sum_i Z_i - 6(\rho_0 + \rho_1 + \rho_2 + \rho_3 + \rho_4 + \rho_5)}{2 + 3 \rho u + 3 \rho u^2} \]

\[ \times \left[ 3.0 + 6 \rho u + 3.0 \rho u^2 \right] \]

\[ \times \left[ 1.5 + 1.5 \rho u + 3.0 \rho u^2 \right] \frac{1}{2} \rho u \]

\[ \times \left[ 3.0 + 6 \rho u + 3.0 \rho u^2 \right] \frac{1}{2} \rho u \]
The slip velocity and temperature jump boundary conditions would be simulated by the specular reflectance bounce back model (combination of bounce back and specular boundary condition) and diffuse scattering boundary condition (DSBC), respectively [40, 44]. For example, the unknown distribution functions along the nanochannel bottom wall are stated as:

\[
\bar{f}_{b,5,6} = \frac{3}{\rho g_e} \bar{g}_{5,6,0} (\rho_u, u_w, e_w) (\bar{g}_{b,5} + \bar{g}_{b,7})
\]

(24)

Naturally the slip velocity and temperature jump along on the nanochannel top wall are simulated similarly.

3.3. Rarefaction and thermal creeping effects

In the nanochannels, the influence of compressibility and rarefaction in the slip flow regime should be involved. Tangential temperature gradients along the nanochannel walls might lead to begin the rarefied gas flows so that the fluid begins creeping in the way from cold place toward hot one. This phenomenon is called thermal creeping or transpiration [3].

According to the several fundamental works of Maxwell [8] and von Smoluchowski [9] over on dynamic of gases, the slip velocity and temperature jump can be demonstrated as follows:

\[
\frac{u_{gy} - u_{wall}}{\lambda} = \left( 2 - \sigma_v \frac{\sigma_v}{\sigma_f} \right) \frac{\partial \theta}{\partial y_{wall}} + \frac{3}{4} \frac{\mu}{\rho_{gy}} \frac{\partial T}{\partial x_{wall}} \quad (T_{gy} - T_{wall})
\]

(25)

\[\sigma_v, \sigma_f\] are the tangential momentum and temperature accommodation coefficients. Dimensionless forms of previous equations are derived using characteristic velocity of \(u_0 = u_t\) and temperature \(T_0 = T_e\), respectively [1, 3]:

\[
U_s = U_s - U_{wall} = \left( 2 - \sigma_v \frac{\sigma_v}{\sigma_f} \right) \frac{\partial \theta}{\partial y_{wall}} + \frac{3}{2} \frac{k - 1}{k} \frac{Kn^2 \Re} {Ec} \frac{\partial \theta}{\partial x_{wall}}
\]

(26)

where \(\sigma_v = \sigma_f = 1, \quad \frac{\partial \theta}{\partial x_{wall}} = \frac{\partial T}{\partial x_{wall}} = \frac{\partial \theta}{\partial x_{wall}}\). The second term in right hand side of Eq. (26) represents the thermal creeping phenomenon which appears to be \(O(Kn^2)\). So this term is usually ignored to determine the slip velocity. However this article claims that it may be important in the nanochannels with tangential temperature gradients on their surfaces.

Moreover, the tangential temperature gradient is suppressed by the prescribed heat flux over the nanochannel surfaces in the literature. In the contrary, present study aims to show the existence and even also significant effects of thermal creeping in a nanochannel with constant temperature over its walls. Eventually the local and averaged Nusselt numbers (\(Nu_x\) and \(Nu_{av}\)) along the nanochannel walls are stated as:

\[
Nu_x = \left( \frac{\partial \theta}{\partial y} \right)_{y=0, y=1}, \quad Nu_{av} = \frac{1}{L} \int_0^L Nu_x \, dx
\]

(27)

4. Validations

The flow and heat transfer of the air nanoflow is simulated using the LBM developed computer code in FORTRAN language. Appropriate grid independency study is performed between 1050 × 35, 1200 × 40 and 1350 × 45 lattice nodes; and among them the lattice with 1200 × 40 nodes shows suitable accuracy and is chosen for the further calculations.

In Fig. 3, the fully developed dimensionless velocity profiles \((U/u_t)\) through a nanochannel are compared with those of Zhang et al. [31] at Kn=0.05 and Kn=0.1 and suitable agreements are observed between them. To have more validation, temperature profiles of \(\theta = T/T_{inlet}\) at different cross sections of a nanochannel versus the results of Kavehpour et al. [7] are presented in Fig. 4 for Re=0.01, \(T_{wall} = 10, \quad T_{inlet} = 1, \quad Pr = 0.7\) and \(Kn_{inlet}=0.01\); this figure also shows good agreements.

5. Results and discussions

Forced convection of air in a two dimensional nanochannel is studied numerically by using lattice Boltzmann method (Fig. 1). Nanochannel side walls are kept hot while the cold inlet air
Fig. 4. Comparison of temperature profiles, $\theta=T/T_e$, through a channel with those of Kavehpour et al. [7].

Fig. 5. Fully developed dimensionless horizontal velocity profiles, $U$, and dimensionless temperature profiles, $\theta$, along the vertical centerline of nanochannel at $\text{Ec}=0.1$ and $\text{Re}=100$ for different values of $\text{Kn}$.

Fig. 6. Profiles of $U$ along the nanochannel at $\text{Ec}=0.1$, $\text{Re}=1000$ and $\text{Kn}=0.001$.

Fig. 7. Profiles of $\theta$ along the nanochannel at $\text{Kn}=0.1$, $\text{Ec}=0.1$ and $\text{Re}=100$.

Fig. 8. Streamlines (top) and Isotherms (bottom) at $\text{Re}=100$, $\text{Kn}=0.01$ and $\text{Ec}=0.1$.

Fig. 9. Streamlines (top) and Isotherms (bottom) at $\text{Re}=10$, $\text{Kn}=0.01$ and $\text{Ec}=0.1$. 
and dimensionless temperature profiles, \( \theta = (T - T_c)/ (T_H - T_c) \), along the vertical centerline of nanochannel at \( Ec = 0.1 \) and \( Re = 100 \) for different values of \( Kn \) are shown in Fig. 5. For the state of \( Kn = 0.001 \) which almost implies to the continuum regime, the maximum of \( U \) occurs at horizontal centerline (at \( Y = 0.5 \)) with the amount of \( U_{\text{max}} = 1.5 \) with ignorable slip velocity adjacent to the walls (at \( Y = 0 \) and \( Y = 1 \)). More \( Kn \) corresponds to more slip at these areas which leads to less \( U_{\text{max}} \). In the other hand, higher \( Kn \) causes lower values for \( \theta \) near the walls and on the horizontal centerline that mean less heat exchange between the fluid and walls.

Fig. 6 illustrates the variations of \( U \) profiles at different cross sections along the nanochannel at \( Ec = 0.1, Re = 1000 \) and \( Kn = 0.001 \). The fully developed condition would occur later at more values of \( Re \) as well as \( X = 0.9L \) where this condition has not been achieved yet in. So it can be mentioned that in the state of \( Re = 1000 \), the whole nanochannel domain is under developing (not fully developed) where the most temperature gradient between the air and walls existences. In the following, the inlet air warming up due to heat exchange with the hot walls is reported in Fig. 7 which concerned at \( Kn = 0.1, Ec = 0.1 \) and \( Re = 100 \).

Figs. 8 and 9 present the streamlines and isotherms for \( Kn = 0.01 \) and \( Ec = 0.1 \) at \( Re = 100 \) and \( Re = 10 \), respectively. Streamlines are completely smooth and symmetric along the horizontal centerline except in a small place at entrance region of left hand side of nanochannel. Fig. 9 shows that the whole space of nanochannel (for \( X > 3.5 \)) is almost in thermal equilibrium with the walls at \( Re = 10 \) while the isotherms of Fig. 8 related to \( Re = 100 \), do not follow such this process; so more length is needed to achieve the isothermal condition.

5.2. Effects of Eckert number

Fig. 10 shows the effects of \( Ec \) on \( U \) profiles along the nanochannel at \( Re = 1000 \) and \( Kn = 0.1 \). It is observed that \( Ec \) affects the velocity profiles significantly at adjacent to walls in entrance region (see the plots related to \( X = 0.2L \)); so that \( U \) profiles far from the inlet do not change sensible with \( Ec \).

Variations of dimensionless slip velocity, \( U_s \), along the nanochannel wall at different values of \( Ec \) and \( Kn \) for \( Re = 100 \) are provided in Fig. 11. \( U_s \) begins from its maximum amount at inlet and then decreases along the nanochannel so that it tends to a constant value at fully developed part of nanochannel. More focus implies that how important is the effect of \( Ec \) on \( U_s \) for the state of \( Kn = 0.1 \) (at \( X < 4 \)); as well as less value of \( Ec \) corresponds to more \( U_s \). The both effects of \( Re \) and \( Ec \) on the profiles of \( U_s \) are presented.
In Fig. 12. As it is said the lower amount of Ec would correspond to a higher value of \( U_s \); although this fact occurs more severely at \( \text{Re}=100 \) than the mode of \( \text{Re}=10 \). Moreover the results concerned \( \text{Ec}=10 \) and \( \text{Ec}=1 \) are more similar to one another than those of \( \text{Ec}=0.1 \). It is worth noting that the negative effect of Ec on \( U_s \) is more sensible at larger Kn.

The higher values of temperature jump, \( \theta_s \), are achieved at entrance region where the most temperature gradient between the cold air and hot wall exists (see Fig. 13). Along the nanochannel, flow approaches to the isothermal pattern with increasing the heat exchange; so the amount of \( \theta_s \) would be
negligible far from the inlet. However $\theta_s$ increases with Kn which means more length will be required to become fully developed. Moreover the positive effect of Re to increase the local Nusselt number ($Nu_s$) and thermal entrance length can be obviously traced in Fig. 14.

Eventually the values of averaged Nusselt number ($Nu_{av}$) versus all of Kn, Ec and Re are seen in Fig. 15. Higher Re and lower Kn increase $Nu_{av}$ and also the effects of Ec can be ignored. However the lowering effect of Kn is more significant at $\text{Kn}=0.1$ than the states of $\text{Kn}=0.001$ and $\text{Kn}=0.01$.

6. Conclusion

Forced convection of air in a two dimensional nanochannel was studied numerically by using the lattice Boltzmann method. Nanochannel side walls were kept hot while the cold inlet air streamed along them. The calculations were performed for $\text{Re}=10,100,1000$ and $\text{Kn}=0.001,0.01,0.1$ and $\text{Ec}=0.1,1,10$. The effects of slip flow regime (according to Kn) involved thermal creeping (according to Ec) on hydrodynamic and thermal domains were investigated for the first time by the lattice Boltzmann method and the following points were achieved:

1. Thermal creeping was usually ignored to determine the slip velocity in the literature. However this article showed that it might be so important in a nanochannel with tangential temperature gradient on its surface.

2. The tangential temperature gradient was practically supposed by the prescribed heat flux over the solid surfaces. In the contrary, the thermal creeping significant effects were observed clearly at present study in a nanochannel with constant temperature over its walls which meant the temperature jump phenomenon would be able to generate the thermal creeping motion.

3. More Knudsen number ($\text{Kn}$) corresponded to more slip velocity ($U_s$) and temperature jump ($\theta_s$) and less Nusselt number ($\text{Nu}$). It also significantly increased the entrance length.

4. Lower amount of Ec led to higher value of $U_s$. Although the results concerned $\text{Ec}=10$ and $\text{Ec}=1$ were more similar to one another than those of Ec $=0.1$. It was worth noting that the inverse effect of Ec on $U_s$ was more sensible at larger Kn. Moreover Ec affected significantly the slip velocity in entrance region so that $U$ profiles far from the inlet did not change sensible with Ec.

5. The mentioned effects of Ec and Kn on hydrodynamic and thermal domains were severely invigorated at higher values of Reynolds number.

6. According to Eq. (26); thermal creeping strength depends on $\text{Kn}^2\text{Re}/\text{Ec}$. Based on this work results, it is recommended that thermal creeping effects for the range of $\text{Ec} < 0.1$, $\text{Kn} > 0.1$ and $\text{Re} > 100$ take in to account and be included, especially for hydrodynamic properties.

References


