SIMULATIONS OF CONVECTIVE HEAT TRANSFER IN RECTANGULAR MICROCHANNEL USING THERMAL LATTICE BOLTZMANN METHOD

by

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The microfluidics becomes an emerging field of interest due to the advent of micro electro mechanical system. In this work simulations were performed to investigate the heat transfer phenomena in microchannel using the 2-D D2Q9 model of thermal lattice Boltzmann method. It is applicable in the whole range of slip velocity. The slip boundary condition which is combination of bounce and specular reflection was applied along with constant temperature boundary condition. For Knudson number greater than 0.001 (slip flow) fluid show slip at walls of the channel. The Reynolds number was kept at 10, Knudson Number 0.002, and aspect ratio (length/height) of 2. The fluid shows a slip of 8% of free stream velocity which is in the reported range. The resulting local Nusselt number was calculated which is responsible to quantify convective heat transfer. The simulation results were ahown to coraborate well with the analytical solution and empirical relations. Hence thermal lattice Boltzmann method satisfactorily predicted heat transfer and momentum transfer phenomena in microchannel.

Keywords: *microfluidics, thermal lattice Boltzmann method, heat transfer*

Introduction

Microfluidics deals with flow through micrometer size channels (1 micron to 1 mm). Microchannel has smaller volume and mass, high surface area to volume ratio and high heat transfer coefficient due to which heat with high flux is removed efficiently. A rapid progress in the manufacturing and utilization of these micro devices has led to their widespread use for both scientific and the industrial community in a variety of applications. However, the small hydraulic diameter in microchannels is responsible for the large heat flux that leads to a rela-

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tively high pressure drop. The careful attention must be given to balance the flow and heat transfer attributes of microchannel systems. Microchannel mostly classified on the basis of knudsen number which is ratio of mean free path to the characteristic length. Flow with Knudsen number less than 0.001 is lies in continuum region, for 0.001 < Kn < 0.1 in slip region, for 0.1 < Kn < 10 in transition region and for Kn > 10 flow is in molecular region [1]. Lee *et al*. [2] investigated heat transfer in rectangular microchannel in laminar region. They found classical and continuum approach valid in microchannel using entrance effect and boundary condition with an error of 5%. It was found that heat transfer have inverse relation with dimension of the channel. Niu *et al* [3] studied the heat transfer in 2-D microchannels using thermal lattice Boltzmann method (LBM). Diffuse scattering boundary condition was used to study velocity slip and temperature jump. Relation of Knudson number with relaxation time was developed. They observed a decrease in local friction coefficient and Nusselt number with the increase in Knudson number and distance along length. Harms *et al* [4] studied thermal flow in microchannels for single channel and multiple channels experimentally. Effect of Reynolds number on Nusselt number and friction coefficient was measured. Thermal resistance and Nusselt number was found to increase with Reynolds number at the cost of pressure drop. The convective heat transfer in a square cavity with Reynold number 10^6 and Prandtl number 0.71 using lattice Boltzmann discretization scheme was studied by [5]. The maximum temperature and velocity was observed at the center of cavity. The velocity and temperature gradient was found to be large along the vertical and small along horizontal boundary-layers. A disadvantage of this numerical method is that we can use only uniform grid for symmetry [5]. Mufti [6] studied the heat and momentum transfer using LBM in thermal flow in macro-channels. Periodic boundary condition was used which did not showed entrance effect. The results were validated with finite difference and analytical solution. A. Akbarinia *et al* [7] studied developing length in microchannel numerically by solving Navier-Stokes equation. They found developing length was proportional to the Reynold number and its effect was found to be more prominent at high Reynold number. It was observed developing length was increased with knudson number. Hamidi and Ouederni [8] simulated flow in microchannel of different shape using FEM. The effect of structure on developing length, velocity profile, and pressure drop was studied. They observed that structural parameters affect the flow properties. Developing length varied inversely with hydraulic diameter and directly with Reynold number. They proposed a correlation for hydrodynamic length in microchannel. Sochi [9] discussed the mechanism of slip at fluid solid interface. He studied the factors on which slip depend that is surface wettability, roughness, microbubble, absorbed gasses and electric charge. The method to find slip length were also established. Sbragaglia [10] theoretical studied the slip at fluid solid interface. They developed a correlation to determine slip length without considering the nature of slip. A correction factor could also explained lotus effect which was responsible for slip at ultra-hydrophobic surface. However, some effects were not considered which was responsible for slip.

The study of heat transfer phenomena in microchannel experimentally is a challenging task due to unavailability of measuring instruments. This work reports the investigation of convective heat transfer in microchannel using thermal LBM. These simulations were carried out in 2-D rectangular microchannels. The aspect ratio of the geometry is taken as 2. As dimensions of microchannel are small so practically, micro channels have low Reynolds number. The top and bottom walls are kept at constant temperature and slip boundary conditions are applied at top and bottom walls. The 2-D D2Q9 model is used for simulating both flow and energy equation.

Problem description

Hot water at 80 °C entering rectangular microchannel with walls at 20 °C with velocity 0.001 m/s. Length of channel is 120 μm and height of channel is 60 μm. Simulation is performed at Knudson (mean free path/characteristic length) number 0.002 and aspect ratio (height/length). Therefore heat is transferred from the fluid to the channel. Fluid-flow in horizontal direction so there will be no effects of gravity. It is assumed flow steady-state and incompressible. Reynolds number is 10 so flow will be laminar. Physical properties are calculated at average temperature which is 50 °C. Prandtl number (viscosity/thermal diffusivity) calculated is 3.8. The channel is rectangular of aspect ratio (height/length) two. The 2-D momentum and heat transfer is studied at macroscopic level. Flow in microchannel is simulated by using slip boundary condition at top and bottom walls of the channel.

Lattice Boltzmann method

The Boltzmann transport equation written as:

$$\frac{\partial f}{\partial t}+\frac{P}{m}\,\nabla f+\,F\,\frac{\partial f}{\partial P}=\frac{1}{\tau}\left(f^{\text{eq}}-f\right) \tag{1}$$

The terms on left side are advection (streaming) term and right side has collision term. Finite difference and finite volume approach is used to discretize this Boltzmann transport equation. The equilibrium distributions in the lattice Boltzmann equation are of the Boltzmann Maxwellian type. They are derived by applying the *maximum entropy* principle under the constraints of mass and momentum conservations up to second-order accuracy and have the following general form independent of the chosen lattice:

$$f_\alpha^{\text{eq}}=\omega_a\rho\left[1+\frac{\vec{e}\vec{u}}{c_s^2}+\frac{\left(\vec{e}\vec{u}\right)2}{c_s^4}-\frac{\vec{u}\vec{u}}{2c_s^2}\right] \tag{2}$$

where u is the fluid velocity, c_s – the speed of sound and equal to $1/\sqrt{3}$, ω_a – the weighting factor, and e – the lattice velocity. A typical lattice Boltzmann simulation is started from known initial values of density and velocity. Initial distributions f is usually calculated as equilibrium distributions. After this initialization step, each time step consists of the following three steps, the same operation being repeated for all cells in one loop. Calculation of the local macroscopic quantities (density and velocity), Collision and propagation. In the collision step is defined as:

$$\tilde{f}_\alpha(\vec{x},t)=f_\alpha(\vec{x},t)-\frac{1}{\tau}\left[f_\alpha(\vec{x},t)-f_\alpha^{\text{eq}}(\vec{x},t)\right] \tag{3}$$

where $\tilde{f}_\alpha(\vec{x},t)$ shows the post-collision distributions. That means, at each time step, for all fluid points in the computational domain, the values of the distribution functions are updated. In collisions between the particles equilibrium distributions function is calculated at each time step. In the streaming or propagation step, the following equation is satisfied:

$$f_\alpha(\vec{x}+\vec{e}_\alpha,t+1)=\vec{f}_\alpha(\vec{x},t)$$

New distributions are calculated in the collision step and propagated to the nearest neighbour in the direction of the lattice velocity for the values at the next time step. Macroscopic physical properties can be calculated from density distribution function as:

$$\rho=\sum_{i=0}^{n}f_i \tag{4}$$

$$u = \frac{1}{\rho}\sum_{i=0}^{n} f_i \tag{5}$$

Boltzmann's equation for temperature transport is similar to momentum transport equation. Simulation proceed is two steps, collision and streaming along wall boundary conditions. We have already discussed streaming and collision for density distribution function, for temperature distribution function this process is same as explained below. For both cases we use dimensionless temperature. To convert temperature in dimensionless form we need two reference temperatures, one hot, and one cold. Dimensionless temperature is:

$$\theta = \frac{T - T_0}{T_i - T_0} \tag{6}$$

where T_i is the fluid inlet temperature and T_0 – the cold reference temperature. The Boltzmann energy transport equation without source term is given as:

$$\frac{\partial g}{\partial t} + (\zeta\nabla) g = \left(\frac{\partial g}{\partial t}\right)_{\text{coll}} \tag{7}$$

After discretization:

$$g_i\left(x + c_i\Delta t, t + \Delta t\right) = g_i\left(x, t\right) - \frac{1}{\tau_g}\left[g_i\left(x,t\right) - g_i^{\text{eq}}\left(x,t\right)\right] \tag{8}$$

Terms on the left hand side of the equation is streaming term and term on the right hand side is collision. Where τ_g is the relaxation time for internal energy and is calculated from thermal diffusivity, α:

$$\tau_g = 3\alpha + 0.5 \tag{9}$$

The equilibrium internal distribution function can be calculated as:

$$g_i^{\text{eq}} = \rho T \omega_i \left[1 + \frac{3e_i u}{c^2} + \frac{9\left(e_i u\right)^2}{2c^4} - \frac{3uu}{2c^2}\right] \tag{10}$$

where g_i^{eq} is the equilibrium distribution function, ω_i – the weighting factor for different vectors, e_i – the lattice velocity, u – the macroscopic velocity, c – the lattice speed (usually equal to 1), T – the local temperature, and ρ – the local density. This equation contains macroscopic velocity term; that is the main source of convective heat transfer.

Boundary conditions

Boundary conditions in microchannel are different from those of the macro-channel because flow lies in slip region where Knudson number range 0.1 to 0.001. Boundary conditions used in microchannel are Drichlet boundary conditions at inlet (inlet velocity), open boundary conditions at outlet (extrapolated), slip boundary conditions at top wall and slip boundary conditions at bottom wall [11].

Slip boundary condition at bottom wall

Velocity slips in microchannel due to different factors such as hydrophobic behavior, surface roughness, presence of gases and surface charge. Slip velocity can be found by evaluating gradients of velocity at the walls:

$$U_{\text{slip}} = \sigma \text{Kn}\left(\frac{\partial u}{\partial y}\right)_w \tag{11}$$

where Kn is Knudson number which is the ratio of mean free path and height of channel and σ – the diffusive momentum coefficient which defines as the fraction of molecule reflected diffusively and equal to [12]. Slip boundary condition can be considered as a combination of bounce back (no slip) and specular reflection (free slip). The unknown distribution function can be found:

$$F_i\left(x,t\right)=qF_b\left(x,t\right)+\left(1-q\right)F_r\left(x,t\right) \tag{12}$$

where q is the probability of bounce back and is normally chosen as 0.7 [13].

The q is 0 for no slip and 1 for free slip case. The $F_i(x,t)$ is the unknown distribution function, $F_b(x,t)$ – the distribution function for bounce back (no slip), and $F_r(x,t)$ – the distribution function for specular reflection. The slip length at liquid interface is schematically represented in fig. 1.

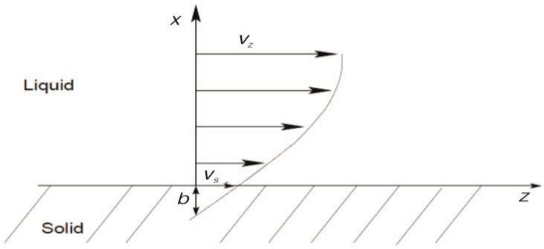

Figure 1. Slip length at liquid solid interface [9]

In fig. 1 V_s is the slip velocity and b is slip length, which is defined to be the imaginary distance where fluid extrapolated velocity approach to zero. In LBM slip length can be evaluated from relaxation time and coefficient of slip ζ where ζ = 1 – q. Slip length will be zero for no slip case (ζ = 0) and infinite for full slip case ($\zeta\to1$). Empirical relation for slip length is given by Nayaz and Hecht [14]:

$$\frac{b}{a}=\frac{\tau\zeta}{3\left(1-\zeta\right)} \tag{13}$$

where b is the slip length, a – the lattice constant, τ – the relaxation time, and ζ – the slip coefficient. The unknown distribution functions F_2, F_5, and F_6 can be find:

$$F_2\left(i,0\right)=F_4\left(i,0\right) \tag{14}$$

$$F_5\left(i,0\right)=q\,F_7\left(i,0\right)+\left(1-q\right)F_6\left(i,0\right) \tag{15}$$

$$F_6\left(i,0\right)=q\,F_8\left(i,0\right)+\left(1-q\right)F_5\left(i,0\right) \tag{16}$$

Slip boundary condition at top wall

Slip boundary condition is also at the top wall of channel applied which is similar to the slip at the bottom wall and unknown distribution functions F_4, F_7, and F_8 can be determine as:

$$F_4\left(i,m\right)=F_2\left(i,m\right) \tag{17}$$

$$F_7(i,m) = qF_5(i,m) + (1-q)F_8(i,m) \tag{18}$$

$$F_8(i,m) = qF_6(i,m) + (1-q)F_7(i,m) \tag{19}$$

Results and discussion

Lattice independent study

As information is passed from one lattice to the other during streaming and collision step so number of lattice should be sufficient to update the information. However, as lattice size increases the required computation also increases so large lattice size requires more computation time and power. Lattice independent study is carried out to check after how many lattice solution become lattice independent. The simulation were performed for different lattice size of 40 × 20, 80 × 40, 120 × 60, and 160 × 80 as shown in fig. 2(a). For lattice sizes 40 × 20 and 80 × 40, velocity profiles are not consistent and smooth. In these cases the information is not updated at the end of channel. The velocity profile becomes consistent after lattice size of 120 × 60. Therefore the simulation results become lattice independent after lattice size of 120 × 60. Keeping this in view our onward simulations for microchannel flow 120 lattice along length and 60 lattices along height are used. The velocity profile is found to be a typical parabolic having slip 8% slip of free stream velocity and slip length of 0.95 µm is measured by using probability factor of 0.7 as recommended by Succi [13]. This agrees with Nayaz and Hecht [14] as they recommended slip of 8-10% of free stream velocity. The results are also compared with [15] and show good agreement with error 10%. An analytical solution of velocity profile for microchannel using slip boundary condition at the top and bottom walls is derived by considering that the Navier-Stokes equation is applicable. The velocity is a function of Knudson number and dimensionless distance along *Y*-axis (*y/H*):

$$U_x = \frac{6U_m\left[\mathrm{Kn} + \left(\frac{y}{H}\right) - \left(\frac{y}{H}\right)^2\right]}{6\mathrm{Kn}+1} \tag{2}$$

The resulted velocity profile is compared with the analytical solution and it was found that the simulation results match well with the analytical results with error of 1.25% as shown in fig. 2(b). In order to validate the simulation results they are compared with finite volume method (FVM) and found in good agreement as shown in fig. 2(c). Velocity profiles are plotted at x = 60 lattice points (60 µm midpoint of the channel). As velocity profile obtain by LBM are in better agreement with analytical solution than velocity profile obtain from FVM so LBM give better predictions of the flow behavior than FVM.

Hydrodynamic developing length

The veocity profile is plotted at differnent length along x-axis in order to estimate the developing length [14]. Velocity is plotted at x = 5, x = 15, x = 30, and x = 35 lattice points along length. It was found that the velocity profile is fully developed at x = 30 lattice or 30 micrometers. The streamlines become parrallel to each other after x = 30 lattice which show that after 30 µm velocity along the length for a fix value of height does not changes as shown in fig. 3(a). Results also show same trend when Horizantal component of velocity contour is plotted against length of the channel as shown in fig. 3(b).

In the entrance region there will be both component of velocity but in fully developed region vertical component of velocity become zero. The results are compared with the empirical relation. Shah and London relation gives developing length of 30 µm which is same as our prediction form LBM [16]. Chen suggest 35 µm developing length which shows 14% error from the simulation value which is due to slip of fluid at walls [16]. Developing length for experiment may increase upto 25% due to slip velocity. As water enters in rectangular microchannel at 80 ^{o}C with walls at 20 ^{o}C so the center is hotter than the fluid near walls. Therefore the temperature profile have parabolic behavior as shown in fig. 4.

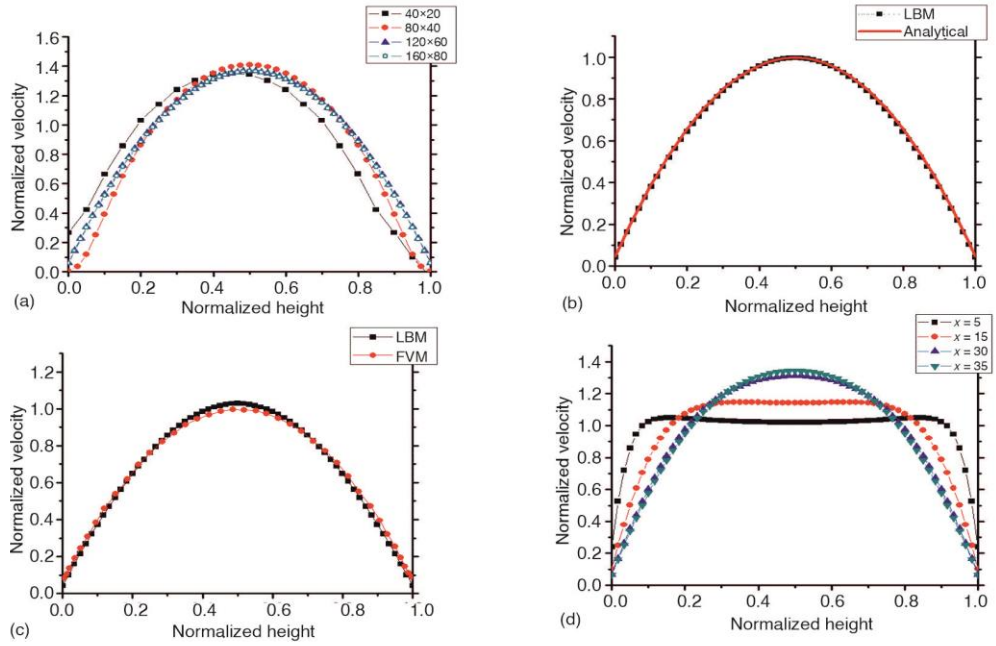

Figure 2. (a) velocity profile at 40×20, 80×40, 120×60, and 160×80 lattice size, (b) comparison of velocity profiles obtained by LBM with analytical solution, (c) comparison of velocity profiles obtained by LBM with those obatained by FVM, and (d) normalized velocity at *x* = 5, *x* = 10, *x* = 30, and *x* = 35 lattice along length

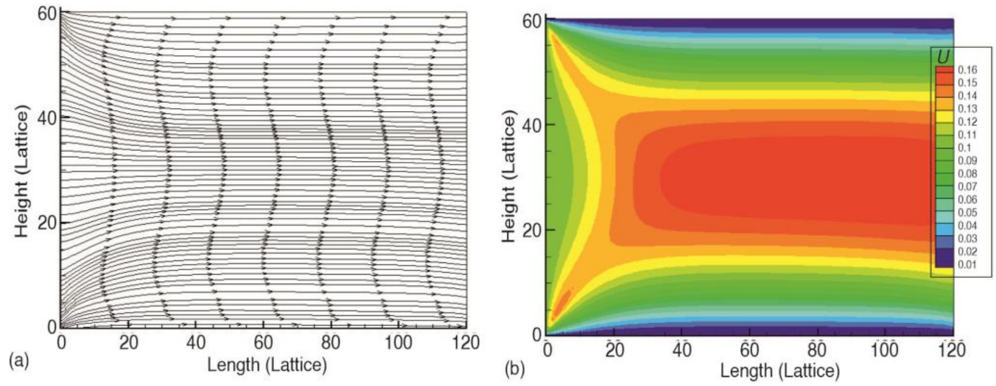

Figure 3. (a) streamlines in rectangular microchannel with Reynold number 10 and (b) contour of horizontal velocity component in microchannel

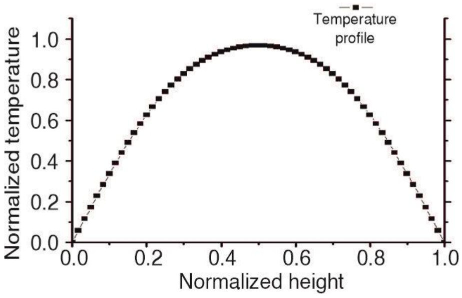

Figure 4. Temperature profile at middle of the channel using LBM

Local Nusselt number

In order to estimate the convective heat transfer we calculate Nusselt number. Nusselt number is ratio of convective heat transfer to the conductive heat transfer. It depends on the heat transfer coefficient of fluid hydraulic diameter of the channel and thermal conductivity of the fluid:

$$\mathrm{Nu} = \frac{hD_H}{k} \tag{21}$$

As hydraulic diameter is in micrometer ranger so it give large heat transfer coefficient which is big advantage the microchannel heat exchanger but at the cost of large pressure drop. Nusselt number depends on the local heat transfer coefficient given as:

$$\mathrm{Nu}_x = \frac{h_x D_H}{k} \tag{22}$$

It can be calculated by finding temperature gradient:

$$\mathrm{Nu}_x = \frac{L_c}{T_w - T_m}\left(\frac{\partial T}{\partial x}\right)_w \tag{23}$$

where L_c is the channel height, T_w – the wall temperature, and T_m – the film temperature and considered as average temperature of the fluid. Nusselt number which is higher at entrance, decreases rapidly with distance then become nearly independent of length. Some empirical relations based on experimental data are developed to evaluate local Nusselt number at different length. Shah and London [16] proposed series of relations for range of Reynold numbers and Prandtl number:

$$\mathrm{Nu}_x = 4.363 + 8.68\left(10^3 x^*\right)^{-0.506} e^{-41x^*} \tag{24}$$

For $x^* > 0.001$ and

$$x^* = \frac{\dfrac{x}{L_c}}{\mathrm{Re}\,\mathrm{Pr}}$$

Local Nusselt number from simulation is compared with the one evaluated from Shah and London [16] as shown in fig. 5(a). Results are agreed well with above empirical relation with 12% error. These predictions are similar with Shah and London [16] other except at start of the channel which may be due to entrance effect. This entrance effect may not be considered properly in the empirical relation. Another relation purposed by Zhuang *et al* [17] to calculate local Nusselt number in the microchannel is given as:

$$\mathrm{Nu}_x = 0.429\,\mathrm{Re}^{0.583}\mathrm{Pr}^{1/3}\left(\frac{x}{2H}\right)^{-0.349}\left(\frac{B}{2H}\right)^{0.494} \tag{25}$$

Local Nusselt number from simulation is compared with empirical values and simulation results shows a good agreement with empirical relation of Zhuang *et al* [17] with an error of 6.5% at the entrance of the microchannel. However, as we move inside the channel these effects diminished and the error was reduced drastically as shown in fig. 5(b).

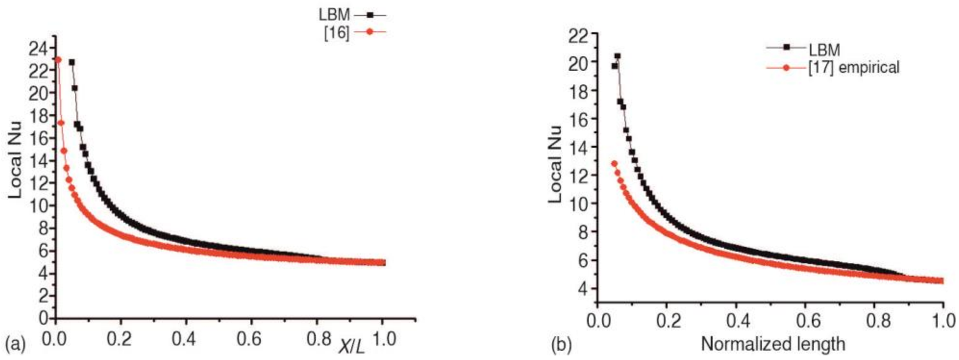

Figure 5. (a) comparison Nusselt number with empirical relation by [16] and (b) comparison of local Nusselt number calculated by LBM with empirical relation [17]

Conclusions

A 2-D convective heat transfer and momentum transfer phenomenon in the rectangular microchannel was simulated using LBM. The slip boundary condition as a combination of the bounce back and specular reflection was applied at the walls of the channel. The probability of bounce back is taken to be 0.7. An 8% of free stream velocity slip was calculated which agrees well with the reported values. The slip at the start of channel was found to be higher which was due to the turbulence effects in the developing region. The developing length was calculated which was found to be 30 micrometer and agreed well with the reported empirical relation. The local Nusselt number was calculated and found to be higher at the start of the microchannel and the becomes approximately constant due to the developed flow. The simulation results were validated by comparing it with the analytical solution, experiment data and FVM and found to be in good agreement with reduced error.

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