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## **Lattice Boltzmann Simulation of Gaseous Flow in Microchannel with Rectangular Grooves**

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### **ABSTRACT**

This paper presents a numerical investigation based on the Lattice Boltzmann method for gaseous flow in a microchannel with rectangular grooves on the walls. Firstly, the prepared computer code is validated with comparison the obtained results with analytic solution for fully developed rarefied gas flow in a simple micro channel. The effects of the rectangular grooves on the flow characteristics and heat transfer behavior are discussed and the results are compared with a simple microchannel. For this purpose, a two-dimensional constant wall temperature microchannel with air as the coolant is investigated. The results show that the heat removal increases for the grooved channel more than 50% compared with a simple microchannel. But the pressure drop is also increases due to the effects of grooves. The increase in friction factor is more than twice for some Knudsen numbers.

### **NOMENCLATURE**

$Kn$  Knudsen number  
 $Pr$  Prandtl number  
 $Nu$  Nusselt number  
  
 $L$  Length of channel  
 $H$  height of channel  
 $h$  height of groove  
 $w$  Length of groove

$s$  distance between grooves  
 $\rho$  Density  
 $\vec{u}$  velocity vector  
 $R$  gas constant  
 $U_0$  average velocity  
 $T$  temperature  
 $T_0$  wall temperature  
 $T_m$  Bulk temperature  
 $q$  heat flux  
 $\rho\epsilon$  Internal energy  
 $D_h$  Hydraulic diameter  
 $\Delta P$  Pressure drop  
 $f$  Friction factor  
  
 $c$  Lattice speed  
 $\delta t$  Time step  
 $\delta x$  Lattice space  
 $f_i$  Hydrodynamic distribution function  
 $f_i^{eq}$  Hydrodynamic equilibrium distribution function  
 $g_i$  Thermal distribution function  
 $g_i^{eq}$  Thermal equilibrium distribution function  
 $\tau_t$  Momentum relaxation time  
 $\tau_g$  Thermal relaxation time  
 $\nu$  Kinematic viscosity  
 $c_s$  Speed of sound  
  
 $x$  Coordinate in x direction  
 $y$  Coordinate in y direction

## INTRODUCTION

Recently due to the rapid development of the micro-electro-mechanical systems (MEMS), study of fluid flow and heat transfer in micro-devices have become an important area of researches. Small dimensions of micro-sized systems cause a distinct character in fluid flows. This physical phenomenon is related to the characteristic length scale, which is defined as Kn number. In MEMS, molecular mean free path is comparable with the characteristic length scale so Kn number is not small and continuum hypothesis breaks down. For  $0.001 \leq Kn \leq 0.1$ , which is referred to slip-flow regime, the no-slip boundary condition is not valid and the gas flow has slip motion and temperature jump at the solid surfaces. Fortunately, Navier-Stokes equations are valid in the slip flow regime so gas flow in this regime can be simulated using the slip boundary conditions [1,2]. Nowadays particle-based methods such as Lattice Boltzmann method is the best choice for modeling high Kn number flows. The Lattice Boltzmann method is an attractive and effective method to simulate gas flow in microchannels because of its intrinsic kinetic [1,3].

As the development of electronic devices has been increased, the heat transfer in these devices has become an attractive topic and many researchers have focused on this field. Alamyane et al. [4] used Lattice Boltzmann method to simulate a channel with extended surfaces for laminar flow regime. They investigated the effect of different parameters on heat transfer enhancement such as Reynolds number, extended surfaces height and spacing. They found that heat transfer was enhanced by increasing Re number and decreasing the objects spacing. Also formation of vortices both in front and behind the objects can enhance heat transfer rate.

Moussaoui et al. [5] studied two-dimensional flow and heat transfer enhancement in a horizontal channel with an inclined square cylinder for different Re numbers. They found that Lattice Boltzmann method can capture physical phenomenon even with a coarse mesh. Also they obtained that heat transfer and Nu number increase strongly as a function of Re number. Abouali and Baghernezhad [6] used arc and rectangular grooves in the floor and sidewalls for heat transfer enhancement in a microchannel. They found that grooved microchannel can remove more heat compared with simple microchannel and arc grooves have better effect on heat transfer removal compared with rectangular grooves. Also an optimum size and spacing for the grooves was presented.

Yan et al. [7] experimentally investigated the effects of surface-mounted short obstacle on heat transfer enhancement in a plate. Three cross-sectional shapes of obstacles, different Reynolds numbers, various numbers of obstacles and obstacle spacing was tested. The results show that heat transfer is enhanced well, when the height of obstacles are half of the channel height. In an experimental study, Chandra et al. [8] investigated fully developed turbulent flow in a square channel with ribbed walls. Different numbers of ribs and various Reynolds number were tested. They found that as the number of ribs increases, the heat transfer coefficient and friction factor increase too.

Eiamsa-ard and Promvong [9] numerically investigated two-dimensional turbulent flow in a channel with grooves on the lower channel wall. Varying Reynolds numbers and groove-

width was investigated. The results reveal that channel with grooved-walls can increase heat transfer at about 158% over the simple channel.

So fabricating grooves for enhancing the heat transfer is a verified approach in microchannels and usual channel sizes. This idea was not tested before for gas flow in microchannel with rarefied gas condition.

In this paper, we use Lattice Boltzmann method to simulate gas flow and heat transfer in a two-dimensional microchannel with rectangular grooves on top and bottom walls. The effect of grooves on heat transfer enhancement and friction factor will be discussed.

## PROBLEM DEFINITION

Figure 1 shows the geometry of the problem. Rectangular grooves are located at the top and bottom walls of the microchannel, which are kept at constant temperature. Cold air stream flows through the channel. The Prandtl number is taken as 0.72 and Reynolds number is 14.5. The channel aspect ratio is fixed at  $L/H=10$ , the ratio of groove's height to the grooves distance is 0.4, the groove's height to the channel's height ratio ( $h/H$ ) is 0.14 and the length of the grooves are two times of their distance ( $w = 2s$ ).

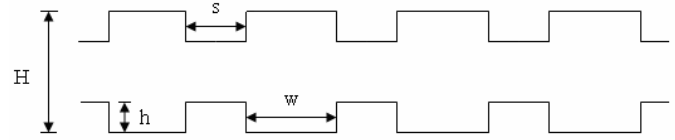


Figure 1. Grooved microchannel's geometry.

## NUMERICAL SIMULATION

The lattice Boltzmann method, which was proposed in 1980s, is a new particle-based numerical method for fluid mechanics simulations. In this method, the macroscopic variables such as velocity, pressure and temperature are not solved directly and a mesoscopic simulation model is used. To apply this method, the fluid domain is discretized in regular square cells or lattices. Each lattice is connected to its neighbors by some links, Figure 2. In the widely used D2Q9 model [6], there are eight links and fluid particles are moved only to its eight immediate neighbors with eight different velocities:

$$c_i = \begin{cases} 0, & i = 0 \\ \left( \cos\left[\frac{(i-1)\pi}{2}\right], \sin\left[\frac{(i-1)\pi}{2}\right] \right) c, & i = 1, 2, 3, 4 \\ \sqrt{2} \left( \cos\left[\left(i-5\right)\frac{\pi}{2} + \frac{\pi}{4}\right], \sin\left[\left(i-5\right)\frac{\pi}{2} + \frac{\pi}{4}\right] \right) c & i = 5, 6, 7, 8 \end{cases} \quad (1)$$

Where  $c$  is the lattice speed and determined by  $\delta x / \delta t$ , and  $c_0$  shows the moving particles with zero velocity, which remain at the node.

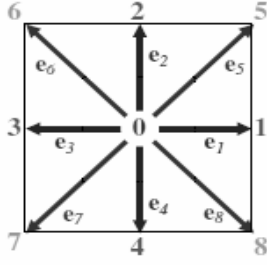


Figure 2. LBM D2Q9 model

In the lattice Boltzmann method the macroscopic quantities are obtained in terms of distribution functions  $f_i(\mathbf{x}, t)$ , which can be calculated by solving Boltzmann equation. The Boltzmann equation describes how the distribution functions  $f_i$  are re-distributed after an interaction [4]. Based on the BGK model this equation is formulated as

$$f_i(x_\alpha + c_i \delta t, t + \delta t) - f_i(x_\alpha, t) = -\frac{\Delta t}{\tau_f + 0.5 \Delta t} [f_i(x_\alpha, t) - f_i^{(eq)}(x_\alpha, t)] \quad (2)$$

$\delta t$  is the time step and  $\tau_f$  is momentum relaxation time.  $f_i^{eq}$  models the equilibrium distribution functions, which can be calculated with

$$f_i^{(eq)} = w_\alpha \cdot \rho \cdot [1 + \frac{3}{c^2} c_\alpha \cdot \vec{u} + \frac{9}{2c^4} (c_\alpha \cdot \vec{u})^2 - \frac{3}{2c^2} \vec{u} \cdot \vec{u}] \quad (3)$$

$w_\alpha$  is weighting factor that depends on the LBM model, for example for D2Q9 model  $w_\alpha$  is determined as follow,

$$\begin{cases} w_i = 4/9 & i = 0 \\ w_i = 1/9 & i = 1, 2, 3, 4 \\ w_i = 1/36 & i = 5, 6, 7, 8 \end{cases} \quad (4)$$

The physical fluid properties such as density and velocity can be described by the distribution functions as follows:

$$\rho = \sum_{i=0}^8 f_i \quad ; \quad \rho \vec{u} = \sum_{i=1}^8 f_i c_i \quad (5)$$

For thermal part of the problem, the governing equation for internal energy density distribution function  $g_i$  is written as:

$$g_i(x_\alpha + c_i \delta t, t + \delta t) - g_i(x_\alpha, t) = -\frac{\Delta t}{\tau_g + 0.5 \Delta t} [g_i(x_\alpha, t) - g_i^{(eq)}(x_\alpha, t)] \quad (6)$$

Where  $\tau_g$  is the thermal relaxation time. In this equation the values of compression work carried out by pressure and viscous heat dissipation are neglected.  $g_i^{eq}(x, t)$  is the corresponding equilibrium state in  $i$ -th direction:

$$g_0^{eq} = -w_0 \left( \frac{3\rho \epsilon u^2 + v^2}{2c^2} \right) \quad (7)$$

$$g_{1,2,3,4}^{eq} = -w_i \rho \epsilon \left( 1.5 + 1.5 \frac{\vec{c}_i \cdot \vec{u}}{c^2} + 4.5 \frac{(\vec{c}_i \cdot \vec{u})^2}{c^4} - 1.5 \frac{u^2 + v^2}{c^2} \right) \quad (8)$$

$$g_{5,6,7,8}^{eq} = -w_i \rho \epsilon \left( 3 + 6 \frac{\vec{c}_i \cdot \vec{u}}{c^2} + 4.5 \frac{(\vec{c}_i \cdot \vec{u})^2}{c^4} - 1.5 \frac{u^2 + v^2}{c^2} \right) \quad (9)$$

In these equations the weighting factor  $w_i$  is the same as Eq. (4). The internal energy,  $\rho \epsilon$ , and heat flux are calculated in terms of internal energy density distribution function  $g_i$ :

$$\rho \epsilon = \sum_i g_i \quad (10)$$

$$\vec{q} = \left( \sum_i c_i g_i - \rho \epsilon \vec{u} \right) \frac{\tau_g}{\tau_g + 0.5 \Delta t}$$

And finally the temperature field can be obtained by  $\rho \epsilon = \rho R T$ , where  $R$  is the gas constant.

The most important dimensionless parameter in simulating microflows, is Kn number, so in the Lattice Boltzmann method first the relationship between Kn number and the relaxation time should be defined. In the kinetic theory, the kinematic viscosity varies linearly with the mean free path:  $\nu = 0.5 \bar{c} \lambda$ , where  $\bar{c}$  is the mean molecule velocity and is given by  $\bar{c} = \sqrt{8RT/\pi}$ . In the Lattice Boltzmann method, kinematic viscosity is determined by  $\nu = (\tau - 0.5)c_s^2 \Delta t$ , where  $c_s$  is the speed of sound. Using these two kinematic viscosities leads to a relation for Kn number for D2Q9 Lattice model:

$$Kn = \sqrt{\frac{\pi}{6}} \frac{\tau - 0.5}{H \cdot \Delta t} \quad (11)$$

$$Kn = \sqrt{\frac{\pi}{6}} \frac{\tau_g - 0.5}{H \cdot \Delta t} Pr$$

### Boundary Condition

As mentioned before, Navier-Stokes equations even with slip boundary condition can be used for small deviation from thermodynamics equilibrium, i.e. for kn less than 0.1. In order to consider rarefaction effects, the Maxwell slip model has been widely used as the boundary condition at the walls. The first-order slip velocity and temperature jump boundary conditions, which were proposed by Maxwell, follow as [16]:

$$u^{slip} = \sigma Kn \left( \frac{\partial u}{\partial y} \right)_w, \quad (12)$$

$$T^{jump} = \phi \left( \frac{2\gamma}{\gamma + 1} \right) \left( \frac{Kn}{Pr} \right) \left( \frac{\partial T}{\partial y} \right)_w$$

Where  $Pr$  is the Prandtl number and  $\gamma$  is the specific heat ratio.  $\sigma = (2 - \sigma_v) / \sigma_v$  and  $\phi = (2 - \sigma_T) / \sigma_T$ ; the tangential momentum accommodation coefficient  $\sigma_v$  is defined as the fraction of molecules that are reflected diffusively, and  $\sigma_T$  is the thermal accommodation coefficient. In the Maxwell model, the accommodation coefficients are free parameters that depend on fluid-solid interface properties and must be determined experimentally, so we have no prior knowledge on the values of these two coefficients [14-17]. Additionally, the Maxwell slip boundary conditions are not appropriate for higher Knudsen number flow ( $Kn > 0.1$ ). Another problem arises when the temperature jump is taken into account; increasing or decreasing the heat transfer with increasing rarefaction, depends on the ratio of the two free parameters: the momentum and thermal accommodation coefficients, which must be chosen empirically; so Reynolds analogy is not preserved any more [15,16].

To avoid aforementioned problems, recently the Langmuir slip model based on the surface chemistry theory has been suggested. In this model the interfacial interaction between the gas molecules and the surface molecules are taken into account.

Gas molecules are assumed to reside on the solid surface for a short period of time via a long range attractive force and after some time lag, these molecules may reflect from the surface. From the macroscopic point of view, this residence time can be interpreted as the degree of wall slip. Consequently in the Langmuir slip model the velocity slip and temperature jump can be expressed as [14-16,18,19]

$$u^{slip} = (1 - \alpha) u_g + \alpha u_w \quad (13)$$

$$T^{jump} = (1 - \alpha) T_g + \alpha T_w$$

The subscript  $w$  stands for the wall and subscript  $g$  represents a local value adjacent to the wall; for example mean free path away from the wall or a reference value such as free stream condition. Coefficient  $\alpha$  depends on the type of the gas and wall material. For monatomic gases it follows as [16],

$$\alpha = \frac{\beta p}{1 + \beta p} \quad (14)$$

And for diatomic gases [16],

$$\alpha = \frac{\sqrt{\beta p}}{1 + \sqrt{\beta p}} \quad (15)$$

where

$$\beta = \frac{1}{4\omega Kn} \quad (16)$$

According to these expressions  $\alpha$  varies with pressure  $p$ , Kn number and coefficient  $\omega$ , which is similar to the slip coefficient in Maxwell model but it can be determined with a clear physical explanation before simulations. It is clear that  $\alpha \rightarrow 1$ , when  $Kn \rightarrow 0$  and  $u_{slip} \rightarrow u_w$ . In present study we choose  $\omega = 1/4$  and  $p = 1.0$ .

Now implementation of Langmuir slip model for the Lattice Boltzmann method will be demonstrated. Before streaming step, some of the distribution functions are unknown and should be determined by boundary conditions. The internal energy and density distribution functions in  $c_2$ ,  $c_5$ ,  $c_6$  direction for lower wall and in  $c_4$ ,  $c_7$ ,  $c_8$  direction for upper wall are unknown. According to the Chapman-Enskog method the density and internal energy distribution functions can be separated in to parts: the equilibrium part and non-equilibrium part [16],

$$f_i(x, t) = f_i^{eq}(x, t) + f_i^{neq}(x, t), \quad (17)$$

$$g_i(x, t) = g_i^{eq}(x, t) + g_i^{neq}(x, t)$$

Here the expressions are written for unknown density and distribution functions in  $c_2$  direction for illustration. Other unknown distribution functions can be handled in the same way. Let  $O$  be the boundary node,  $W$  be the wall node and  $B$  be the nearest fluid node to the boundary node. The post collision distribution functions can be assumed as [16]

$$f_2(O, t) = F_2^{eq}(O, t) + (1 - \eta_f) F_2^{neq}(O, t), \quad (18)$$

$$g_2(O, t) = G_2^{eq}(O, t) + (1 - \eta_g) G_2^{neq}(O, t)$$

where

$$\eta_f = \frac{\Delta t}{\tau_f + 0.5\Delta t} \quad (19)$$

$$\eta_g = \frac{\Delta t}{\tau_g + 0.5\Delta t}$$

According to the Langmuir slip model, the natural choices for  $F_2^{eq}(O, t)$  and  $G_2^{eq}(O, t)$  are

$$F_2^{eq}(O, t) = \alpha f_2^{eq}(W, t) + (1 - \alpha) f_2^{eq}(B, t), \quad (20)$$

$$G_2^{eq}(O, t) = \alpha g_2^{eq}(W, t) + (1 - \alpha) g_2^{eq}(B, t)$$

and

$$F_2^{neq}(O, t) = \alpha f_2^{neq}(W, t) + (1 - \alpha) f_2^{neq}(B, t), \quad (21)$$

$$G_2^{neq}(O, t) = \alpha g_2^{neq}(W, t) + (1 - \alpha) g_2^{neq}(B, t)$$

$f_2^{eq}(B, t)$  and  $g_2^{eq}(B, t)$  are both known since macroscopic quantities of the flow such as velocity, temperature and mass density are known at the fluid node  $B$ . For  $f_2^{eq}(W, t)$  and  $g_2^{eq}(W, t)$ , the velocity  $u(W, t)$  and temperature  $T(W, t)$  are both known while  $\rho(W, t)$  is unknown. To handle this, using  $\rho(B, t)$  instead of  $\rho(W, t)$  is suggested [16]

$$f_2^{eq}(W, t) = f_2^{eq}(\rho(B), u(W), T(W), t), \quad (22)$$

$$g_2^{eq}(W, t) = g_2^{eq}(\rho(B), u(W), T(W), t)$$

For non-equilibrium part of the distribution functions at node  $B$  we can write

$$f_2^{neq}(B, t) = f_2(B, t) - f_2^{eq}(B, t), \quad (23)$$

$$g_2^{neq}(B, t) = g_2(B, t) - g_2^{eq}(B, t)$$

and the non-equilibrium distribution functions at node  $W$  can be approximated as [16]

$$f_2^{neq}(W, t) = f_2^{neq}(B, t) = f_2(B, t) - f_2^{eq}(B, t), \quad (24)$$

$$g_2^{neq}(W, t) = g_2^{neq}(B, t) = g_2(B, t) - g_2^{eq}(B, t)$$

Substitute Eq. (23) and (24) into Eq. (21) we have

$$F_2^{neq}(O, t) = f_2(B, t) - f_2^{eq}(B, t), \quad (25)$$

$$G_2^{neq}(O, t) = g_2(B, t) - g_2^{eq}(B, t)$$

and finally Eq. (18) becomes

$$f_2(O, t) = \alpha f_2^{eq}(\rho(B), u(W), T(W), t) + (1 - \alpha) f_2^{eq}(B, t) + (1 - \eta_f) [f_2(B, t) - f_2^{eq}(B, t)] \quad (26)$$

$$g_2(O, t) = \alpha g_2^{eq}(\rho(B), u(W), T(W), t) + (1 - \alpha) g_2^{eq}(B, t) + (1 - \eta_g) [g_2(B, t) - g_2^{eq}(B, t)]$$

## VALIDATION OF NUMERICAL MODEL

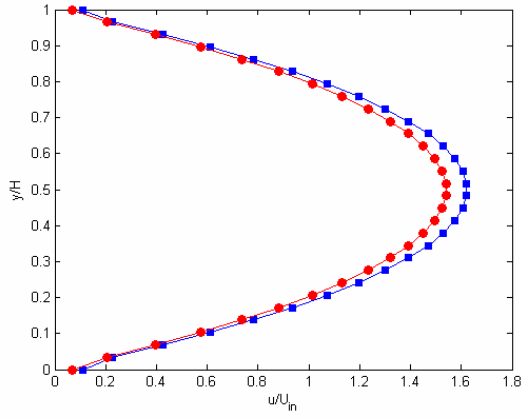
In order to validate our numerical model, a two-dimensional simple microchannel is simulated using Lattice Boltzmann method. A cold air is forced through the channel and the walls are kept at constant temperature. Figures 3 and 4 show comparison between velocity and temperature profiles of present work and related analytical solutions resulted by solving Navier-Stokes and temperature equations with slip and no-slip boundary conditions [5]

$$u(y) = 6U_0 \left[ \left( \frac{y}{H} \right) - \left( \frac{y}{H} \right)^2 + Kn \right] \quad (27)$$

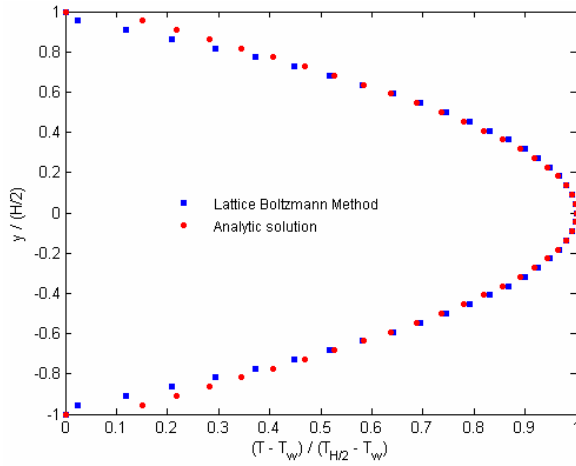
$$\frac{T_0 - T}{T_0 - T_m} = \frac{3}{16} Nu \left( \left( \frac{y}{H/2} \right)^2 - \frac{1}{6} \left( \frac{y}{H/2} \right)^4 + \frac{5}{3} \right) \quad (28)$$

$$T_0 - T_m = (T_0 - T_{in}) \exp \left( - \frac{\alpha Nu}{U_0 H^2} x \right) \quad (29)$$

Where  $U_0$  is average velocity,  $T_0$  is the wall temperature;  $T_m$  is the bulk temperature of the stream and  $\alpha$  is the thermal diffusivity.



**Figure 3. Velocity profile of micro-Poiseuille flow: solid line, analytical solution; square,  $Kn = 0.02$ ; circle,  $Kn = 0.01$**

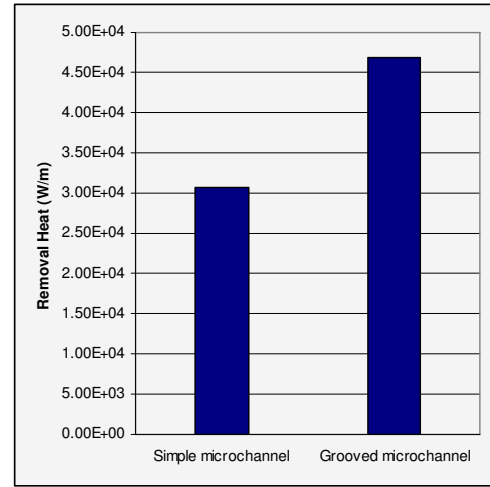


**Figure 4. Temperature profile of Poiseuille flow:  $Kn < 0.001$**

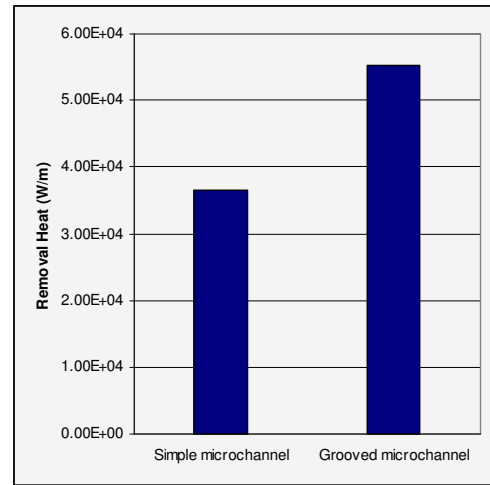
As the figures 3 and 4 show, the developed numerical model is in complete agreement with analytical solutions and this confirms the validity of the developed computer code.

## RESULT AND DISCUSSION

In this section, the numerical results of the Lattice Boltzmann simulation for two values of the Knudsen number:  $Kn = 0.015$  and  $0.02$  are presented. Figure 5 and Figure 6 compare heat removal for simple microchannel and grooved microchannel at  $Kn = 0.015$  and  $0.02$ . As the results show, the heat removal of the grooved microchannel is 50 % more than that for a simple microchannel.



**Figure 5. Comparison between removal heat of simple and grooved microchannel at  $Kn = 0.015$**

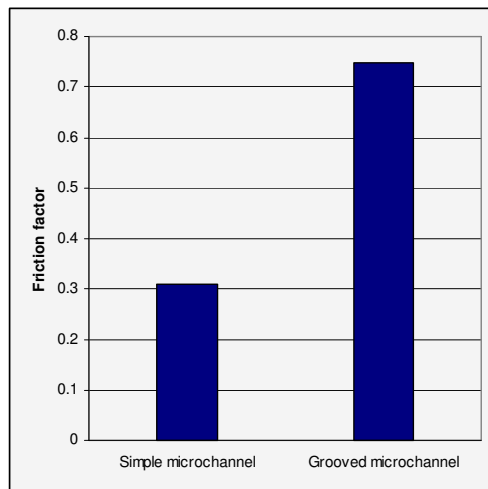


**Figure 6. Comparison between removal heat of simple and grooved microchannel at  $Kn = 0.020$**

Although adding rectangular grooves to a simple microchannel enhance the heat transfer but causes increasing of pressure drop and friction factor too. The friction factor is described as

$$f = \frac{\Delta P}{(4l/D_h)1/2(\rho U_{in}^2)} \quad (30)$$

Figure 7 compares friction factor for simple and grooved microchannel at  $Kn = 0.015$ . According to this figure rectangular grooves on top and bottom walls cause higher pressure drop compared with simple microchannel. So care must be taken to balance heat transfer enhancement and added friction factor. Increase of the pressure drop due to the grooves is more pronounced for smaller  $Kn$  numbers. The friction factor increases to more than twice for  $Kn = 0.015$ .



**Figure 7. Comparison between friction factor of simple and grooved microchannel at  $Kn = 0.015$**

## CONCLUSION

In this paper the laminar gas flow and heat transfer for slip regime in a two-dimensional grooved microchannel is investigated numerically using the Lattice Boltzmann method. Rectangular grooves are located on the top and bottom walls which are kept at constant temperature. Boundary conditions for slip velocity and temperature jump are applied at the walls. The effects of  $Kn$  number and rectangular grooves on heat transfer enhancement and friction factor of the microchannels are also studied. The results show that adding rectangular grooves at microchannel's walls, increase heat transfer and friction factor compared with a simple microchannel.

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