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SIMULATION OF THE FLOW AND THE STUDY OF THE EFFECTS OF THE SURFACE ROUGHNESS IN ISOTHERMAL GAS FLOWS OF MICRO SCALE USING LATTICE BOLTZMANN METHOD

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ABSTRACT

In this paper, a lattice Boltzmann method used in the simulation of the fluid flow in micro/nano scale is introduced and studied. The method can be employed instead of NS equations in cases where the continuum assumption is no longer valid. In the present study the aim is to investigate the effects of surface roughness on flow characteristics of micro/nano gas flows. In order to compare the final results, two flow geometries were chosen for which the numerical and experimental results were available. Surface roughness was increased in each stage (from completely smooth to 12% roughness) and its influences on the flow regime, pressure and velocity distribution, slip velocity and mass flow rate were studied. It is shown that surface roughness results in a decrease in the mass flow rate as well as slip velocity. Increasing the amount of roughness causes the mass flow rate to continually decrease, however this trend is inverted for the slip velocity.

Keywords: Micro Flow, Nano Flow, Surface Roughness

INTRODUCTION

Micro nano systems are being increasingly investigated by many researchers. Since nearly all micro devices operate in a fluid media, the understanding of flow phenomena at the micro level is fundamental to the development of MEMS & NEMS. Features such as film damping of resonant structures, viscous forces, heat transfer in mass flow sensors have to be understood before an effective and optimized design of micro devices can be made.

While the mechanical properties of some micro devices are reasonably well studied, the research on micro flows is still at a preliminary stage. The main reason behind this is that at tiny-level, the continuum assumption is no longer valid since the mean free path of gas molecules is the same order as the typical geometric dimension of the device.

Continuum assumption on which the Navier–Stokes (NS) equations are based is valid only when the characteristic length L of the system is much larger than the mean free path λ of the molecules. The kn number which is defined as the ratio of λ to L ($Kn = \lambda / L$) can suitably be used as a measure of applicability of the NS.

In many cases involving macroscopic flows, the Kn is indeed small ($Kn \leq 0.001$). However, there are now increasingly many applications where Kn is relatively large. In a micro-scale channel or Micro Electro Mechanical Systems (MEMS), for instance, Kn can reach or exceed 0.1 depending on the characteristic length of interest, given $\lambda = 65nm$ for air at room temperature. High Kn flows may also occur in low pressure vacuum devices or at high altitude. For $Kn \geq 0.001$, the continuum assumption is no longer valid and modifications to the NS are necessary.

Based on the Kn number of the flow, the flow can be classified into a number of regimes: continuum flow, $Kn \leq 10^{-3}$; slip flow, $10^{-3} \leq Kn \leq 10^{-1}$; transition flow $10^{-1} \leq Kn \leq 10$ and free-molecular flow, $Kn \geq 10$.

The lattice Boltzmann method (LBM) is a powerful CFD tool that can be used for the simulation of the flow in different regimes. It has received considerable attention by fluid dynamic researchers over the past two decades.

The guiding principle of the LBM is to construct a dynamic system on a regular lattice involving a number of the single particle distribution functions of fictitious particles on the links of the lattice. The particles then evolve in a discrete time according to certain rules which guarantee the satisfactions of some desirable macroscopic behaviors, e.g., compressible thermal or isothermal fluids, emerging at scales larger than the lattice spacing.

While the number of particles distributed in the computational field is strongly related to the number of molecules in Molecular dynamics and Direct Simulation of

Monte Carlo methods, the LBM uses a fixed lattice that makes it more computationally efficient than MD and DSMC methods in many cases.

Also, since the LBM solver is based on a simplified kinetic model, namely the lattice Boltzmann equation (LBE), the use of a complicated scheme to solve the full BE is usually avoided.

It should be noted that the LBM is directly derived from microscopic principles, and so it could present a natural tool for studying rarefied gas dynamics. Other advantages of LBM include its scalable performance in a parallel computing environment, coding simplicity, and robustness in dealing with complex boundary conditions. LBM has already had substantial impact on fundamental research and engineering applications involving hydrodynamics of small, moderate and high-*Kn* flows.

Many investigators have studied the small-scale flow phenomena using LBM in recent years. Nie et al. [1] employed the lattice Boltzmann method to simulate a 2D flow in a micro channel. They studied the effects of gas rarefaction using a Kn-related molecular relaxation frequency. The impact of gas rarefaction on pressure distribution curvature in a micro channel was investigated by Lim et al[2], where they used a local pressure dependent Kn number. A comparison of the results with Arkilic et al. [3] was also given in their study. Gas-solid interface behavior was studied by Zhang et al. [4] utilizing tangential momentum accommodation coefficient. Niu et al.[5] performed a simulation of the Poiseuille and Couette flow in a micro channel geometry and investigated the effects of boundary condition type on pressure drop and mass flow rate in the flow.

In the present study, the written FORTRAN code has the ability to simulate the flow in micro nano scale using the lattice Boltzmann method. The written code has a flexible structure which has the advantage that it can be readily developed by future researchers. The aim in this study is to investigate the effects of surface roughness on flow parameters such as pressure distribution, slip velocity and mass flow rate.

THE NUMERICAL ALGORITHM

The most common form of the lattice Boltzmann equation (LBE) is :

$$f_i(r + c_i.\delta t, t + \delta t) - f_i(r,t) = \Omega_i(f) \qquad (1)$$

where f_i are the particle density distributions defined for a finite set of discrete particle velocity vectors $\boldsymbol{c}_i : i = 0, \ldots, b$. These particle speeds define links among nodes on a given lattice. The collision term on the right side of Eq. (1) often uses the so-called Bhatnagar–Gross–Krook (*BGK*) approximation,

$$\Omega_i(f) = -\omega(f_i - f_i^{eq}) \qquad (2)$$

With a single relaxation frequency ω. Here, f_i^{eq} is the local equilibrium distribution function that has an appropriately prescribed functional dependence on the local hydrodynamic properties. The basic hydrodynamic quantities, such as fluid density ρ and velocity **u** are obtained through moment summations in the velocity space,

$$\rho = \sum_0^b f_i = \sum_0^b f_i^{eq} \quad \text{and}$$
$$\rho u = \sum_0^{q-1} e_i f_i = \sum_0^{q-1} e_i f_i^{eq} \qquad (3)$$

With an appropriate choice of lattices and suitable f_i^{eq}, the LBE obeys conservation laws of mass, momentum and energy in the physical space and recovers the NSEs for long wavelengths and in the low frequency limit via Chapman–Enskog expansion. The fluid kinematic viscosity ν is uniquely mapped to the relaxation time:

$$\nu = C_s^2\left(\frac{1}{\omega} - \frac{1}{2}\right) \qquad (4)$$

Where for the particular lattice model used here Cs = $(1/3)^{0.5}$ is the adiabatic speed of sound.

It has been shown that solutions of the LBE converge to those of NS for small *Kn* flows (*Kn*≤0.001). At the same time, the LBM is intrinsically kinetic and involves no continuum assumptions. Therefore, in principle, there should be no obstacles for application of the LBM to high *Kn* flows.

The relaxation time τ ($= 1/\omega$) is normally assumed to be a constant, which is acceptable for nearly incompressible flows. For high *Kn* flows, however, the global density variation can be large. Nie et al. [1] proposed to replace the relaxation frequency ω in Eq. (2) by ω' :

$$\frac{1}{\omega'} = \tau' = \frac{1}{2} + \frac{1}{\rho}\left(\tau - \frac{1}{2}\right) \qquad (5)$$

Using the Chapman–Enskog multi-scale expansion technique, they obtained the following relation:

$$\nu = \frac{C_s^2}{\rho}(\tau - \frac{1}{2}) \qquad (6)$$

Implying that the dynamic viscosity μ = ρν is constant which might be considered to be more realistic.

For an ideal gas modeled as rigid spheres, the mean free path λ is related to the viscosity ν as:

$$\nu = {}^1\!/_2\, \nu_m.\lambda \qquad (7)$$

Where the mean velocity of the molecular defined as:

$$\nu_m = \sqrt{{}^{8K_BT}\!/_{\pi m}} \qquad (8)$$

m represents the molecular mass and K_B is the Boltzmann constant.

Hence, form equations (4), (7) and (8), we get:

$$Kn = \frac{\lambda}{H} = \frac{2\nu}{\nu_m H} = \sqrt{\frac{\pi}{6}}\frac{\tau - 0.5}{N_H} \quad or \quad \tau = \frac{Kn\, N_H}{\sqrt{{}^{\pi}\!/_{6}}} + \frac{1}{2} \qquad (9)$$

Where N_H is the lattice number in the channel height, *Kn* is local Knudsen number.

Since, the mean free path is inversely proportional to the pressure, the local *Kn* can be calculated by:

$$Kn = \frac{Kn_o.P_o}{P_{(x,y)}} \quad (10)$$

Where Kn_o and P_o are the Kn and the pressure at the outlet. Therefore, in equation (9), τ is variable along the channel.

The boundary conditions applied to the numerical algorithm are in a way which makes the inlet and outlet velocities fully-developed. By fully-developed it is meant that the velocity profiles at inlet and outlet boundaries are parabolic and there is no need to consider a developing length at the inlet. The pressure at these boundaries is held fixed for a number of different constant values. The initial pressure distribution in the computational domain (between the inlet and outlet boundaries) is assumed linear in order to accelerate convergence. The Bounce Back boundary condition is considered for the walls while a specific velocity boundary condition is not applied to the walls so that the slip velocity the Kn number increment are simulated directly.

FLOW AND GEOMETRY CHARACTERISTICS

Two model geometries present in the previous experimental and numerical studies were chosen for the investigations. The first geometry is based on the study of Pong et al. [6] that has been referred to and used for verification by many previous researchers such as Chen et al. [7] in 1998 and Reni [8] in 2003. These two investigators compared the results of a finite element simulation using a modified boundary condition with those of Pong et al. The micro channel used in the first model is 3000 micron in length and 1.2 micron wide.

The second case is based on an experiment performed by Arkilic et al. [4], with *H=1.33 μm* and *L=75000 μm.*

Five different pressure ratios are used between 1.34 and 2.70, based on outlet pressure, yielding a maximum Knudsen number of 0.0585 (slip regime) for first case and 0.155 (transition regime) for second case.

The model dimensions and gas properties for two cases of simulation are listed in Table 1.

Table 1. Dimensions and Properties of Fluid

	Case I	*Case II*
Fluid	Nitrogen	Helium
L (μm)	3000	7500
W (μm)	40	52.25
H (μm)	1.2	1.33
P_{in}/P_{out}	1.34 – 2.7	1.34 – 2.7
P_{out}*(kPa)*	100.8	100.8
T (K)	314	314
Kn_{out}	0.0585	0.155
K	1.4	1.667
R (J/kg.K)	296.7	2076.9

We used 3 different roughness percentages (4%, 8% and 12%) in the modeling of fluid flow in rough channels; Fig 1 shows the velocity profiles in a micro channel with 8% surface roughness. An increase in the value of velocities in the direction of flow is noticeable in this figure. For both studies cases we also used LBM for smooth wall condition in order to compare the results.

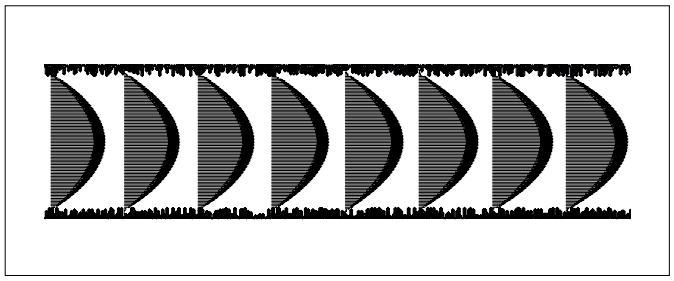

Fig 1. Velocity profiles in a micro channel with 8% surface roughness

RESULTS AND DISCUSSION

Figs. 2 and 3 compare the pressure distribution along the channel for rough channel with 4% roughness with experimental data of Pong et al. [6] (case I) and numerical data of Reni [8] (case II), respectively. The increasing in nonlinearity of pressure distribution is clear in these figs.

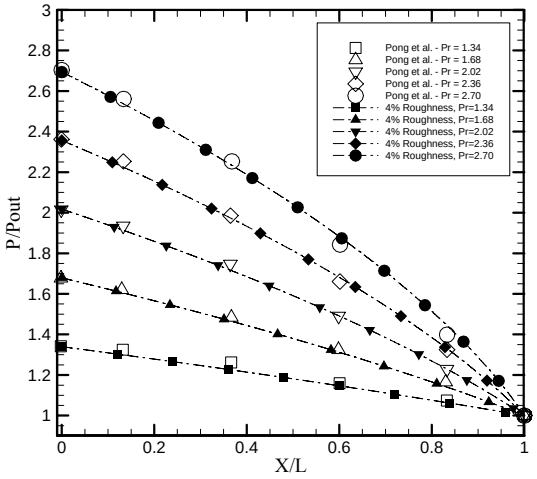

Fig 2. Comparison of pressure distribution for 4% roughness with experimental data of *Pong et al.*

Fig. 4 shows LBM results of the normalized pressure deviation from the linear pressure distribution for smooth and 4% rough channel for different pressure ratios.

By comparing the smooth and the rough channel results we can see about 20% increase in the curvature of pressure distribution for the first studied case.

Fig. 5 shows the pressure distribution for 4% roughness for the second case compared with the numerical results of Reni [8] . The normalized pressure distribution in the second case for smooth and rough channels is shown in fig.6. The results represent about 60% increase in pressure curvature for this case. These results demonstrate that the effects of surface roughness are increase as Kn number increases.

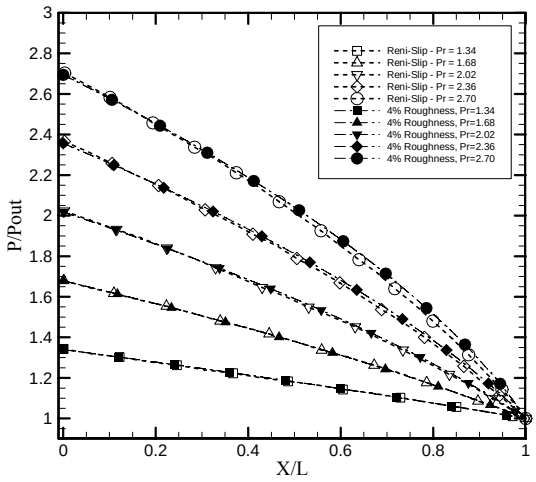

Fig 3. Comparison of pressure distribution for 4% roughness with numerical data of *Reni. Case I*

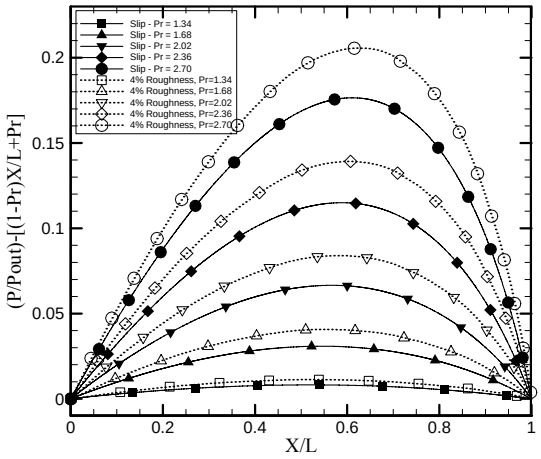

Fig 4. Comparison of normalized pressure distribution for 4% roughness with LBM results for smooth channel. *Case II*

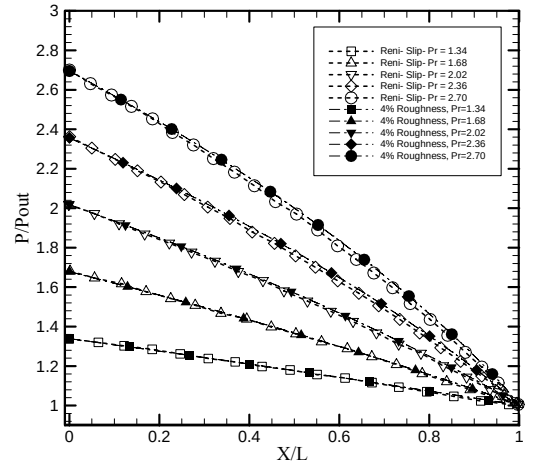

Fig 5. Comparison of pressure distribution for 4% roughness with numerical data of *Reni. Case II*

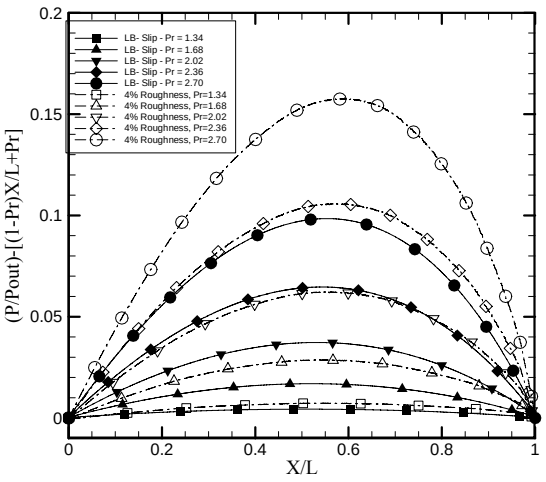

Fig 6. Comparison of normalized pressure distribution for 4% roughness with LBM results for smooth channel. *Case II*

Figs. 7 and 8 represent the center line velocity along the channel length for cases I and II, respectively. In case I the roughness causes about 12% decrease in velocities in comparison with the smooth channel. The surface roughness in the second case causes about 65% reduction in velocity values and this reduction implies the stronger effect of roughness in higher Kn numbers again.

Figs. 9 and 10 show the effect of roughness on slip velocities for two cases respectively; Results show the noticeable reduction for slip values in both cases. Another comparison for slip velocities between different roughness percentages are demonstrated in Figs. 11 and 12. These results are noteworthy; for both cases the results show that the slip velocity increases as the amplitude of roughness increases. The reason behind this behavior is the formation of micro vortexes among roughness that keep the bulk of the fluid away from the wall.

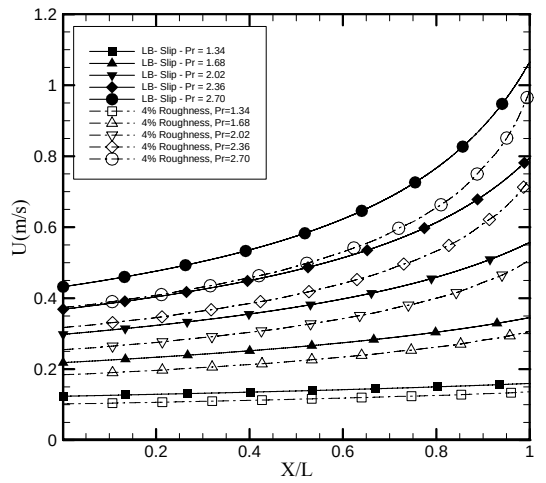

Fig 7. Comparison of centerline velocity distribution for 4% roughness with LBM results for smooth channel. *Case I*

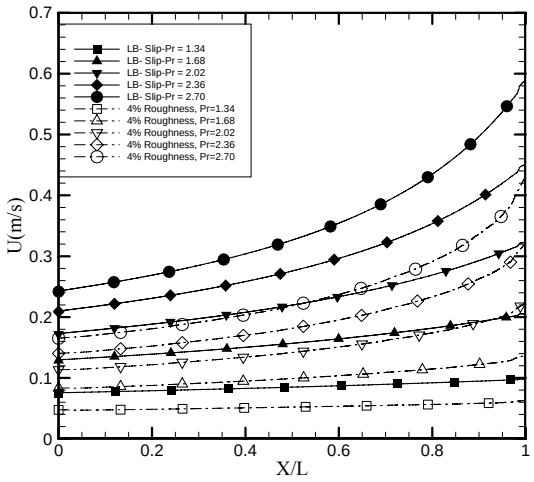

Fig 8. Comparison of centerline velocity distribution for 4% roughness with LBM results for smooth channel. *Case II*

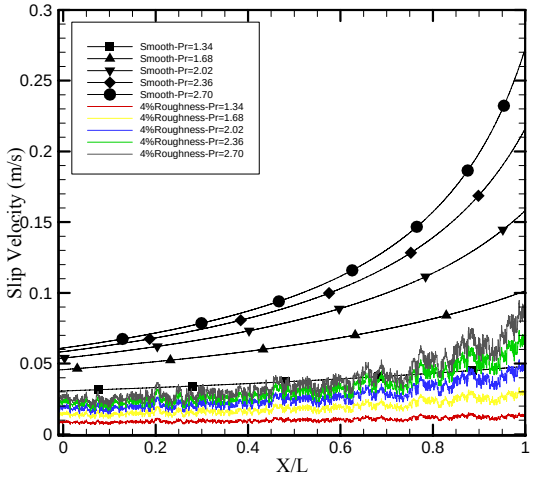

Fig 9. Comparison of slip velocity distribution for 4% roughness with LBM results for smooth channel. *Case I*

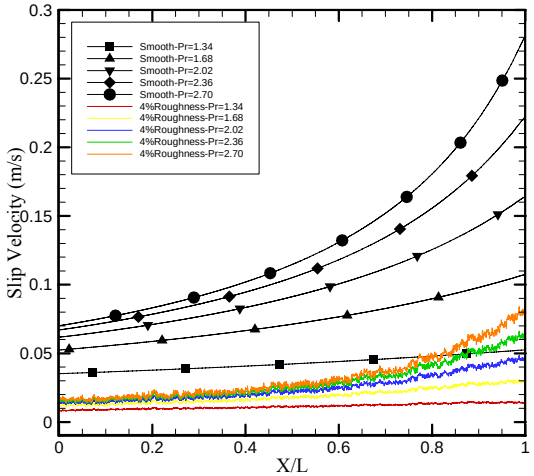

Fig 10. Comparison of slip velocity distribution for 4% roughness with LBM results for smooth channel. *Case II*

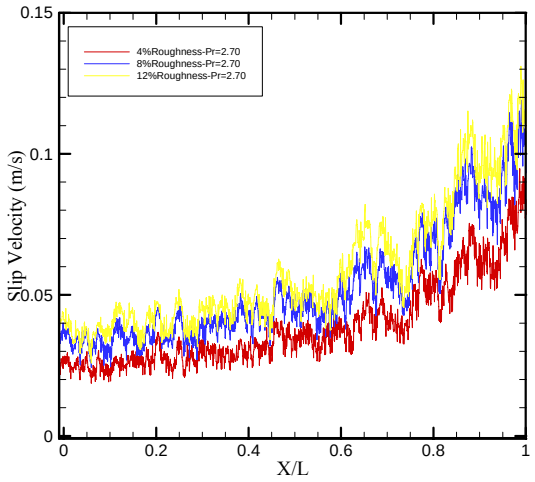

Fig 11. Effect of different roughness percentages on slip velocity distribution. *Case I*

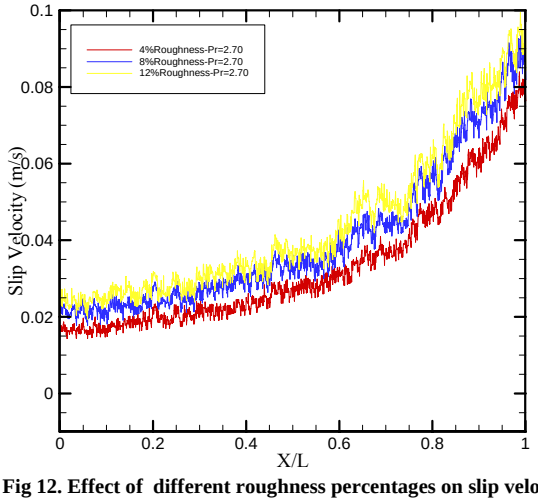

Fig 12. Effect of different roughness percentages on slip velocity distribution. *Case II*

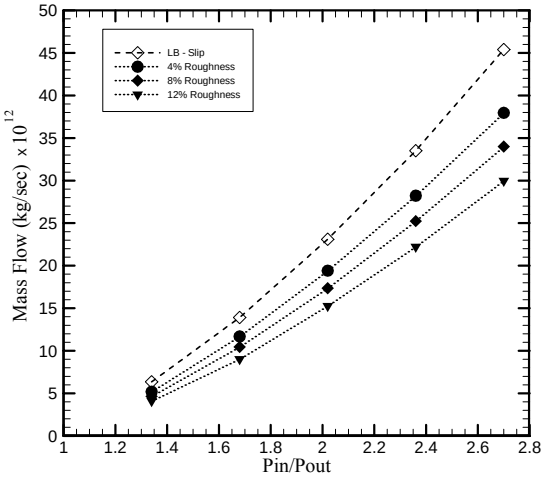

Fig 13. Effect of different roughness percentages on mass flow rate. *Case I*

Finally the effect of different roughness in mass flow rate of cases I and II are shown in figs. 13 and 14, respectively. The results shows the maximum reduction of about 25% for the first case mass flow rate and 50% reduction for the second one.

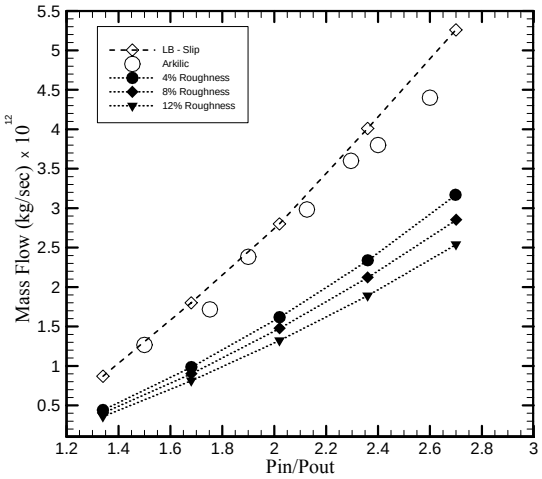

Fig 14. Effect of different roughness percentages on mass flow rate. *Case II*

CONCLUSIONS

The advantage of the LBM is that it can readily be used for the analysis of the flow in complex geometries. The method is suitable for exploitation in a wide range of nano /micro electro mechanical systems, and other nano technological applications related to high *Kn* number cases. The present study shows that the LBM is an effective and appealing numerical simulation tool for the microflows.

Regarding the comparison of the results and the provided discussions, the following final conclusions can be obtained:

1. Surface roughness causes an increase in the curvature of pressure distribution in channel.
2. Surface roughness results in a reduction in the bulk and slip velocity of the fluid.
3. Surface roughness causes reduction in mass flow rate of fluid flow.
4. The percentage of the effect of roughness on the flow parameters depends on roughness percentage, pressure ratio of channel and the Kn number at the outlet of channel.
5. Increasing of the pressure ratio causes an increase in the effect of roughness on flow parameters.
6. An increase in the surface roughness causes a reduction in the mean velocity and mass flow rate and increases the slip velocity.

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