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EFFECTS OF SURFACE ROUGHNESS PERIODICITY AND CHANNEL HEIGHT IN NANO-CHANNEL FLOWS

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ABSTRACT

One of important phenomenon's in micro and nano-devices is slippage. The concept of slip length has been introduced to compute slip at the solid surfaces. A large slip length decreases dissipation at the surfaces and results in changing pressure drop. In this paper, the effect of roughness periodicity has been studied, which deals with distances between corrugations, on velocity profile and slip length variations by molecular dynamics simulations. To have a perfect analysis, the channel walls was chosen to be rough and after that by increasing the distances between corrugations which result in increasing periodicity of roughness, its effect on variation of velocity profiles undergoing Poiseuille flow was investigated. Also, the slip length in each simulation which shows the magnitude of slippage was calculated. As the results showed, when roughness periods increased, velocity profiles were found to be the same as flat channel's profile and slip length decreases. The outcomes also reveal a non-linear dependency of the slip length magnitude on the roughness period. Slip length profiles also showed that slip decreases by increasing the height of the nano-channel, because solid-fluid interface effects will disappear in channels with more height and slip length would have greater magnitudes as a result.

INTRODUCTION

Analyzing flow at micro/nano scales has a variety of applications such as biomedicine, carbon nanotubes, micro-integrated circuits, etc. Understanding micro and nano-devices is needed to optimize their performance and broadening their applicability. Due to high surface to volume ratios in nanofluidic systems, interfacial effects will be dominated. Slip phenomenon is one of these effects which is important in micro/nano scales. Besides, no slip condition which is a common boundary condition in continuum, will not apply in such scales and continuum models are almost useful up to micro scales.

Increasing slip in channels will increase dissipation in such systems which will increase pressure drop, as known as an undesired phenomenon. Abnormous decrease of drag has a large economic effect in analyzing micro and nano-devices. Although a large amount of experimental data on the slip length exists [1], but because it is difficult to investigate fluid velocity near the liquid/solid, atomistic simulations are preferred. Also due to small scales in nano channel, experimental measurements are practically difficult and atomistic approaches such as molecular dynamics simulations become appropriate.

In molecular dynamics simulations (MD), lagrangian particles trajectories are calculated under force field by newton's second law. This method is definitely exact and will elucidate accurate information of system near solid surfaces and of course it is a meshless method.

To quantify slip in channels, slip length L_s is introduced which is defined as the distance next to the wall at which the extrapolated fluid velocity would be equal to the velocity of the wall and depends on different factors: surface energy, surface roughness, fluid structure and shear rate. Although much experimental tests has already been done, there is much differences between those tests and numerical results. Accurate investigations for velocity profile near solid-fluid interfaces are difficult.

In MD simulations, there isn't any assumption for slip velocity which is an important benefit. In previous studies, the effect of channel height in flat nano/mesoscale channels undergoing Poiseuille and Couette flows was investigated in a majority of studies [2-4]. Both the wall-fluid interaction and surface roughness are important and should be considered simultaneously in determining the nanostructures and profiles of monatomic fluid flow in a nano-channel. The previous simulation showed that the roughness and cavitation of the same dimensions induces different local density pattern while the overall average might be the same [5]. It showed that the maximum value of streaming velocity in the center of the channel is not significantly affected by the presence of roughness and velocity profiles were suppressed in the upper half of the channel where the rough wall is present, while they are similar to those of a smooth channel in the lower half of the channel [6].

In this work, the effects of surface roughness periodicity and channel height effects in rough channels are simulated to investigate velocity and slip length variations. The paper is aiming at understanding slippage with the presence of roughness and variable roughness periodicity.

Innovation of this work is that we consider the effect of roughness periodicity with corrugation of constant amplitude and length. Also channel height effect is investigated in a rough nano-channel undergoing Poiseuille flow.

NOMENCLATURE

T	[K]	Temperature
f	[kg.m/s^2]	Force
K_B	[m]	Boltzmann constant
r	[m]	Distance between particles
x	[m]	Cartesian axis direction
y	[m]	Cartesian axis direction
z	[m]	Cartesian axis direction
Ls	[m]	Slip length
Φ	[J]	Potential function
σ	[m]	Molecular diameter
ε	[J]	Energy parameter
ρ	[g/cm^3]	density

Subscripts

wf	Wall and fluid
ff	Fluid and fluid
ss	Solid and solid
sf	Solid and fluid

MODEL CONFIGURATION AND METHODOLOGY

In this study, Poiseuille flow in rough nano-channel is simulated by molecular dynamics simulation. To better feel fluctuations near interfaces, we chose this method which predicts slip length more accurately. General algorithm of MD simulations described in [7,8]. Calculating intermolecular forces between particles is done by Lennard-Jones(12-6) potential which is [7]:

$$\phi(r) = 4\varepsilon\left[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6} \right] \tag{1}$$

where ε and σ represent the energy and length scales of fluid particles respectively. Liquid argon is chosen for fluid particles with mass per atom (m) as $6.69*10^{-23}$ g, density as $\rho = 0.8\sigma^{-3}$, and molecular diameter as $\sigma = 3.4*10^{-8}$ cm. All of the simulations have been done in non-dimensional units and we chose periodic boundary condition at x and z directions and fixed boundary at y direction. According to the Newton's second law, acceleration expression for each particle is:

$$m\frac{d^2 r_{ij}}{dt^2} = \sum_{i=1, i\neq j}^{N} \frac{\partial\phi}{\partial r_{ij}} \tag{2}$$

where N is the total number of molecules in the simulation. Non-dimensional ratios of the LJ parameters, the relative atom size, σ_r, and the relative energy parameter, ε_r, are defined as follows:

$$\varepsilon_r = \varepsilon_{sf} / \varepsilon_{ff} = \sqrt{\frac{\varepsilon_{ss}}{\varepsilon_{ff}}} \tag{3}$$

$$\sigma_r = \sigma_{sf} / \sigma_{ff} = \sqrt{\frac{\sigma_{ss}}{\sigma_{ff}}} \tag{4}$$

Wall particles consist of two faced-centered-cubic (FCC) layers with the same mass as fluid particles and density of $\rho = 4.0\sigma^{-3}$ with fixed atoms which means that wall atoms do not interact with each other. Throughout the simulations, fluid temperature keeps constant and equal to $T = 1.2\varepsilon/k_B$ which is equal to 132 K. Before the main simulation, an equilibrium calculation is done with $5*10^4$ steps. The time step is $\Delta t = 0.005\tau$, where $\tau = (m\sigma^2/\varepsilon)^{1/2}$ is the LJ time and 10^6 steps are considered for main simulation which is enough to reach a steady flow state with the cutoff radius $r_c = 2.2\sigma$ for fluid-fluid and wall-fluid interactions. Also roughness amplitude is 1σ from the wall surface. The slip length L_s according to its definition can be calculated by:

$$L_s = u_s / (\frac{du_s}{dy})_{y=0} \tag{5}$$

and the dimensionless slip length is defined as $l_s = L_s / H$.

EFFECT OF ROUGHNESS PERIODICITY

In the first stage, we studied the effect of increasing roughness period. The first selected dimensions of the system in x, y and z directions are 20*32*5 σ with amplitude corrugation of 1.5 σ. We selected 5, 6, 8, 10 and 12σ for the distances between corrugations with constant amplitude and height for implementation of roughness. In the first state, distances between corrugations and roughness length are equal and in other states we increased this distance to observe velocity profile's changes. Therefore the distances between corrugations are the only parameter which varies in this part of the simulation. We have shown computational domain of our simulations in this stage in Figure 1.

Three sets of parameters for the wall-fluid interactions are employed which is related to different slip conditions:

(1) $\varepsilon_{wf} = 0.2\ \varepsilon \quad \sigma_{wf} = 0.75\ \sigma$
(2) $\varepsilon_{wf} = 0.4\ \varepsilon \quad \sigma_{wf} = 0.75\ \sigma$
(3) $\varepsilon_{wf} = 0.6\ \varepsilon \quad \sigma_{wf} = 0.75\ \sigma$

External force on each fluid particle is $f_x = 0.05\ \varepsilon/\sigma$ which applies to each particle during simulation and after each time step by applying Newton's second law, new velocity and position particles are calculated.

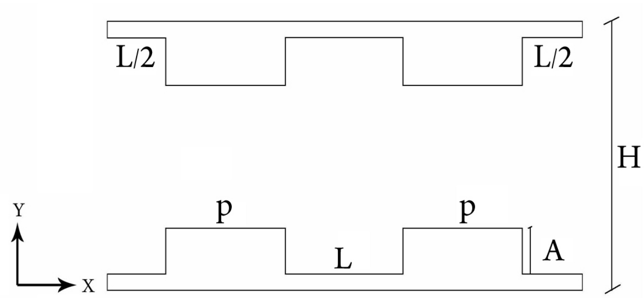

Figure 1 Computational domain: 2corrugations with periodic boundary condition and constant amplitude

Figure 2. displays velocity changing at L=5σ for three interactions. As we can see, increasing the amount of interaction between wall and fluid will result in decreasing slip velocity. This is due to the fact that whenever wall-fluid interaction increases, wall particles will attract fluid particles near the surface more and it results in decreasing slip velocity. This behaviour also decreases the slip length.

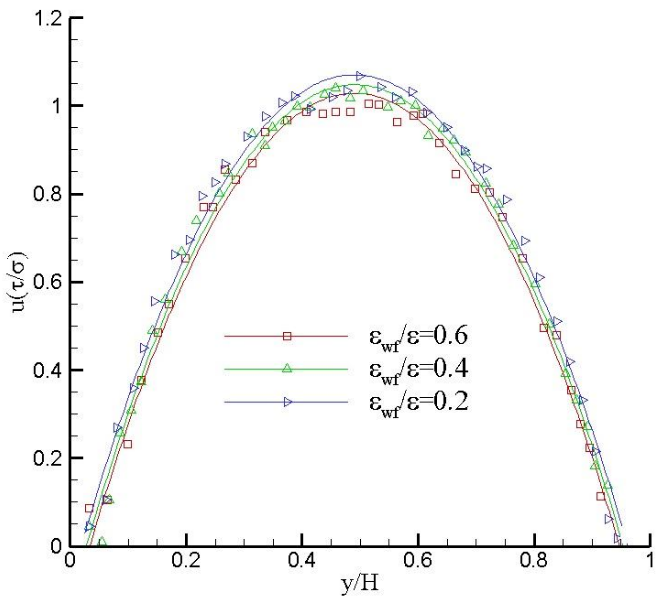

Figure 2 Velocity profile at different wall-fluid interactions and L=5σ

Figure 3. is also displays velocity changing at L=12σ for three interactions. As like as Figure 2, increasing the amount of interaction between wall and fluid will result in decreasing slip velocity. In this state the differences between velocity profiles for three interactions increases compared with the state L=5σ and maximum amount of velocity is also increases. By increasing roughness period and decreasing corrugation effects rough channel tends to flat channel and with constant external force, particles velocities would be greater and as a result maximum velocity increases.

Figure 4. shows velocity profile of four rough walls and one smooth wall within bins of thickness $\Delta z = 0.1\sigma$. As we can see, in rough wall there is a great decrease in slip condition and shows importance of the surface roughness for slippage phenomena. According to this figure, by increasing the period of the roughness, the slip velocity and the peaks of the profiles gradually grow however it decreases in some cases. In fact periodicity increasing is equivalent to decreasing corrugations and wall channels tend to smooth wall and with more increasing periodicity of roughness velocity profiles will be closer to flat state. Therefore, as the roughness decreases the slip phenomenon, we will see the same behaviour by decreasing the roughness period. Also velocity slip increases in this state with respect to state L=5σ and fluid particles near the liquid/solid interface have greater velocity.

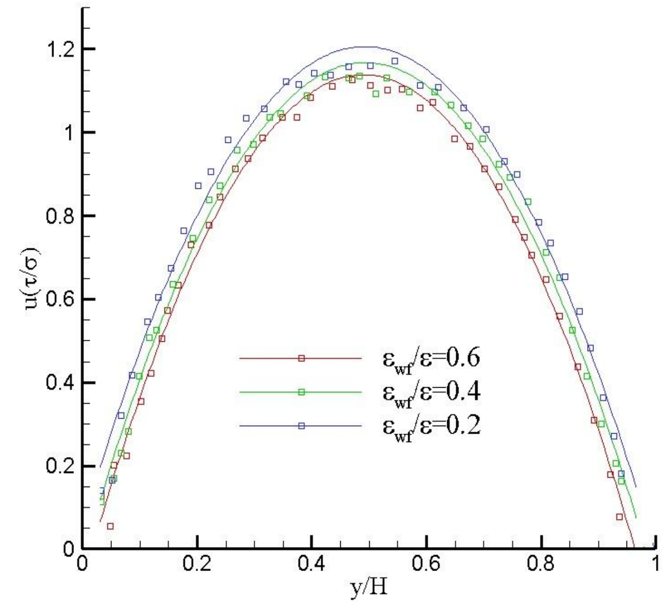

Figure 3 Velocity profile at different wall-fluid interactions and L=12σ

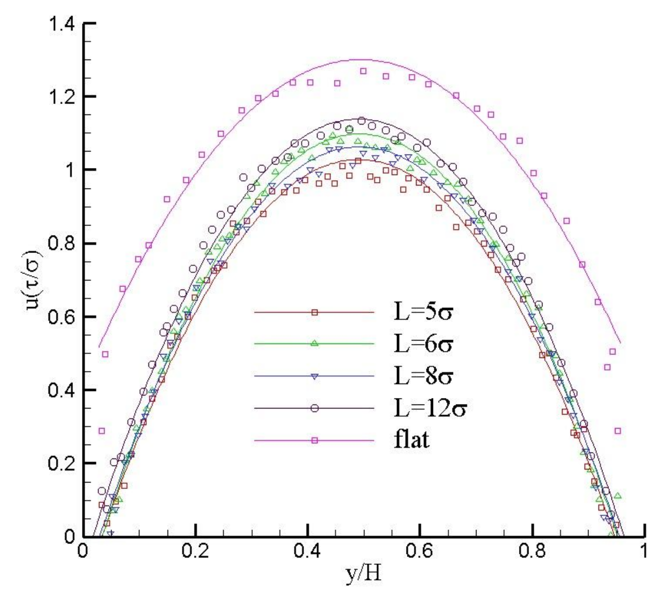

Figure 4 Velocity profile for different periodicity and flat state

It should be noted that Navier-Stokes equation for flows in channel predicts a quadratic equation for velocity. Therefore, we used quadratic curve fitted to the velocity profiles, it is worth noting that MD results have an oscillatory nature with fluctuations especially near corrugation of surfaces.

Slip length behaviour as a function of roughness periodicity at three interactions are shown in Figure 5. As we discussed, decrease of periodicity (increasing L) is equivalent to decrease of the effect of the roughness and decreasing slip length. This is more pronounced with a nonlinearity behaviour and period effect become more drastic at greater amount of L. Also increasing the interaction between the wall and fluid will have an effect on the slip length and will increase it due to the higher mobility of fluid particles near the wall surface.

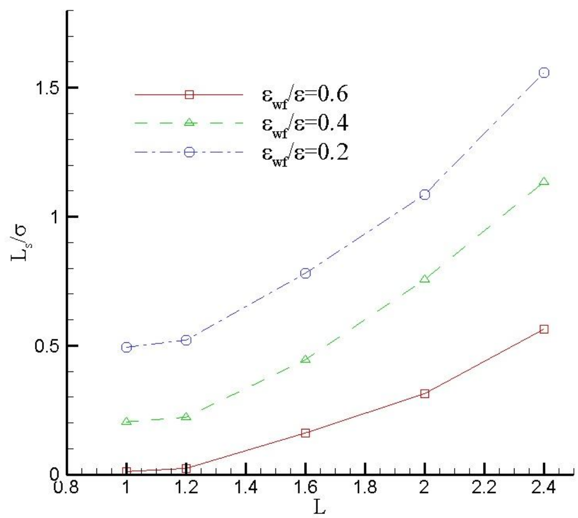

Figure 5 Slip length variation as a function of roughness periodicity at different wall-fluid interaction

EFFECT OF CHANNEL HEIGHT

In this stage the channel height is increased to investigate its effect on the velocity and slip length profiles in a nano-scales rough channel. The channel dimensions in x, y, and z directions are 20*30*5 σ respectively with varying height from 30 σ to 60 σ. LJ parameters are assumed $\sigma_{wf} = 0.75\sigma$ and $\varepsilon_{wf} = 0.6\varepsilon$**,** the external force on each particle is $f_x = 0.02\ \varepsilon/\sigma$ and constant in simulations. In this state we have one corrugation in our simulations with periodic boundary condition at x and z direction.

Velocity profiles for these simulations are shown in Figure 6. By increasing height velocity profile varies greatly and maximum velocity increases with increasing velocity of fluid particles. Also velocity profile changes from quadratic state and fluid particles in the middle of the channel and next to it have almost the same velocity magnitudes and velocity profile is flat next to the middle of the channel at the height of 60σ and slip velocity increases by increasing channel height.

Slip length shown in Figure. 7. According to this figure, by increasing the magnitude of the height, although the roughness effect practically disappears but actually the interface effect cancels out and slip length will decreases. By the way this behaviour in not linearly and slip length decrease will be greater by increasing channel height.

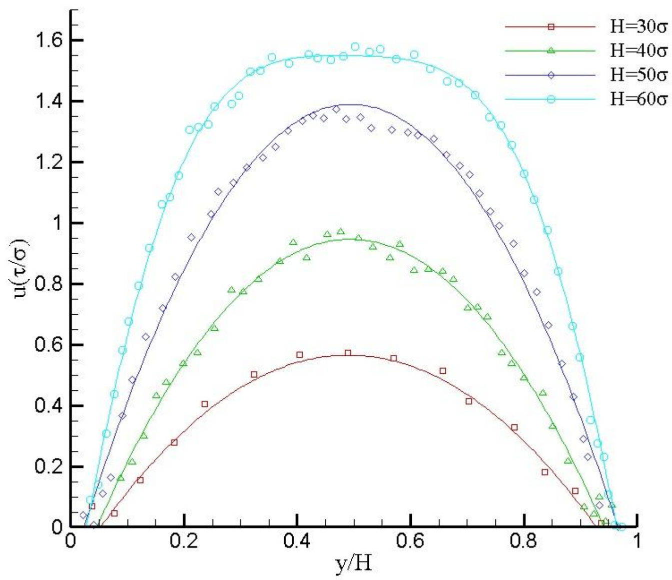

Figure 6 Effect of channel height on velocity profile

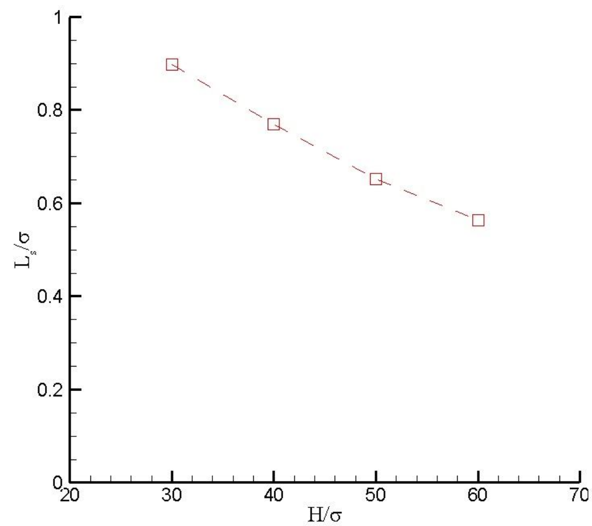

Figure 7 Effect of channel height on slip length

CONCLUSION

In this paper, we used molecular dynamics simulation to study the effect of roughness periodicity on the velocity and slip length. We considered roughness with constant dimension but varying its periodicity. Then, we studied channel height effect in a rough channel with Poiseuille flow. We noticed that by increasing interaction between wall and fluid, slip velocity and slip length will decrease. It was found that when roughness period increases along with more distances between corrugations, slip length will vary nonlinearly and similar to exponential form.

In second stage, by increasing the channel height, we studied its effect on the slippage. According to our results, slip length will decreases and velocity profiles will be more stretched and they tend to their limit at a constant external force. With the height we considered, velocity is very sensitive to height variations. Also, slip length decreases nonlinearly by increasing channel height.

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