



# Molecular dynamics simulation of surface roughness effects on nanoscale flows

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## ABSTRACT

In the present study, a molecular based scheme has been developed for simulating of surface roughness effects on nano- and micro- scale flows. In micro channel flow, there are some differences on the flow friction between roughness and cavitations which are not well studied. In the presented approach, based on the Molecular Dynamics Simulation (MD), the Lennard–Jones potential is used to model the interactions between particles. Particles equation of motion is integrated using fifth order Gear predictor-corrector. Periodic boundary condition is implemented via minimum image convention. Each atom of the solid wall is anchored at its lattice site by a harmonic restoring force and its temperature has been controlled by utilizing Nose-Hoover thermostat.

The roughness is implemented on the lower channel wall. To make a comparison between the effect of roughness and cavitations, the same dimension is used for both with different aspect ratio. To allow comparison with previous results, the same fluid density has been also used.

The effects of surface roughness and cavitations on velocity distribution of hydrophobic and hydrophilic wall undergoing Poiseuille flow are presented.

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## 1. Introduction

In nano-scale flows, molecular structure of the fluid and surfaces, and their interactions between them at the atomistic length scales play a key role, and hence the molecular dynamics (MD) method emerges as a viable approach for investigation of the flow physics in such scales [1–3]. Recent developments in MD simulation of the nanoscale fluid flows are summarized in [4] and [5]. Heat and fluid flow in microchannels are quite different from those in macrochannels. Owing to the high surface to volume ratio, surface affects domain in small devices. The non-slip boundary conditions, which exist in macroscale, are no longer valid in small scale devices, under some circumstances. The interfacial effects on flow and heat transfer on micro/nano scale are discussed in [6].

Previous nanoscale fluid flow MD simulations were focused on velocity slip on the boundary, and they have shown that the boundary slip on the liquid–solid interface is mainly a function of the wall–fluid interaction strength, fluid/wall density and shear rate [7,8]. In previous works, the effects of atomic roughness, wall–fluid interaction and surface wettability on slip lengths and

fluid behavior in nanochannel with different wall-crystal structures were studied. The degree of slip was found to decrease with surface roughness for both the hydrophobic and hydrophilic surfaces.

In order to describe interactions of gas molecules with the surface, Maxwell [9] described specular and diffuse reflection models in 1897, which were appropriate in kinetic theory based approaches [10]. However, many MD simulations use more advanced wall models with fixed lattice structure instead of simple specular walls. Fixed lattice walls consist of wall molecules fixed in their lattice positions and collide (interact) with fluid molecules via intermolecular forces [7,11]. Similarly, instead of fixing the wall molecules in their lattice positions, it is possible to assign very heavy mass (e.g.  $\text{mass}_{\text{wall}} = 10^{10} \times \text{mass}_{\text{fluid}}$ ) to wall molecules, which allows motion of wall molecules based on their interactions with fluid atoms and each other [12]. Since “fixed” lattice wall model impart energy to the system, it is necessary to utilize a thermostat to dissipate viscous heating induced by the shearing motion. A more advanced wall model utilizes a lattice of molecules connected to crystal positions with harmonic bonding. Cieplak et al. [13] examined boundary conditions at the wall–fluid interface using harmonic springs attached to the lattice position of each wall molecule, which allowed the wall molecules to vibrate, emulating the thermal motion of solid crystals. In order to confine the displacements of the oscillating wall molecules, the authors used appropriate stiffness constants for bonding.

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