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Study of fluid flow behavior in smooth and rough nanochannels through oscillatory wall by molecular dynamics simulation

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HIGHLIGHTS

- A simulation for the behavior of Argon flow in oscillatory Couette flow of flat and rough nanochannels has been proposed.
- In this type of flow, the slip length depends on the wall velocity, and the frequency and period of the oscillations.
- Applying rectangular and triangular roughness to lower wall reduces the fluid slip.
- The current study is assumed to be more accurate and comprehensive in comparison with previous studies in oscillating Couette flows.

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ABSTRACT

The method of molecular dynamics simulation is applied in order to study the behavior of liquid Argon flow within oscillatory Couette flows, in both smooth and rough nanochannels. To accomplish this study, the fluid velocity and the fluid slip in oscillatory Couette flows were used to assess the effects of: oscillatory velocity amplitude, speed frequency rate, channel height, wall density, and the amount of interaction between fluid and wall particles. Both smooth and rough walls were modelled in order to investigate the effect on the fluid patterns as well. Rectangular and triangular wall roughnesses in different dimensions were used to study this effect. The results indicate that an increase in the velocity amplitude increases the fluid slip, and decreases the fluid velocity fluctuations near the walls. Similar to the steady-state Couette flow, in oscillatory flow we observe a decrease in fluid slip by reducing the wall density. Moreover, by reducing the energy parameter between the fluid and wall, the fluid slip increases, and by reducing the length parameter the fluid slip decreases. Implementing the rectangular and triangular roughness to the bottom wall in the oscillatory flow results in a decrease in fluid slip, which is also similar to the usual non-oscillating flows.

1. Introduction

In recent years, computational fluid dynamics (CFD) based on numerical calculations have gained great attention. Scientists have found it possible to study different processes more carefully, and have facilitated their enquiries by applying

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Nomenclature

f_i	Force random (N)
k_B	Boltzmann constant (J/K)
m	Mass of molecule (kg)
N_f	Number of fluid particles
N_w	Number of wall particles
r_c	Cutoff radius (nm)
r_{ij}	Inter-particle separation (nm)
T	Temperature (K)
$x_i,\ y_i,\ z_i$	Coordinates of particle
$\ddot{x}_i$	Accelerated particle in the x-direction
$\ddot{y}_i$	Accelerated particle in the y-direction
$\ddot{z}_i$	Accelerated particle in the z-direction

Greek symbols

ε	Energy parameter (J)
ρ	Fluid density (kg/m^3)
ρ_w	Wall density (kg/m^3)
σ	Length for liquid argon (nm)
τ	Time scales

Subscripts

f	Fluid
w	Wall
wf	Wall–fluid
x	x-direction
y	y-direction
z	z-direction

computer simulations. Computer simulations contribute by providing almost exact results for some problems in statistical mechanics, issues that may not be resolved by other methods or merely approximated techniques.

Several methods have been developed and introduced as computer simulation methods. Amongst these, the molecular dynamics simulations including Lagrangian methods perform in specific areas such as interface phenomena, molecular level problems, simple and polymeric fluids, and so on. A few achievements have also been obtained in the analysis of fluid flow in nano and micro scales using molecular dynamics (MD) simulation [1,2], which is considered to be one of the most appropriate methods for nanoscale problems. For this reason, this method is applied in this study. The fluid particles composition, and the interaction between the fluid and wall act as essential effects on the study of fluid flows in nano and micro scales. Therefore, the use of molecular based numerical methods is sufficient and precise in the analysis of engineering problems. For this reason, molecular dynamics simulation is an efficient method with which to study the physical behavior of different flows in such scales [3–5]. The MD simulation can provide detailed information, especially near the boundaries such as the fluid–solid interface, which is the main concern in many applications. Moreover, CFD based methods could not be applied, since the Navier–Stokes equations are not valid in most nanoscale problems. Amongst the many different fluid flow applications, Couette flow is one of the most important and is applied in many microfluidic and nanofluidic devices, including the air flow between computer hard drive plates, high-speed centrifugal pumps, and some micro and nano-pumps.

Many studies are conducted using molecular dynamics simulations in order to study the stable fluid flows under different conditions. Toghraie and Azimian [6] simulated the Poiseuille flow in a nanochannel through non-equilibrium molecular dynamics. They obtained the density, velocity and temperature profiles. In order to obtain a more uniform temperature distribution across the channel, they applied local thermostating near the channel wall. They found that velocity, slip length and slip velocity profiles depend on driving force.

In different types of studies, MD simulations were used to study the stationary flow due to the wetting fluid, and the effect of chemically patterned surfaces on the fluid flow control. These effects are caused by the wetting characteristics of fluid particles, and by the chemical change in the solid surface, which lead to a change in the fluid behavior near the interface of fluid and solid [7,8].

Another type of flow which is very common, and is the focus of the current study, is Couette flow, whereby the flow is driven by shear stress. Lee and Kim [9] simulated the turbulent plane Couette flow for a Reynolds number of 6000. They produced a variety of turbulence statistics, which included all the terms in the transport equations of Reynolds stresses, and the functions of density due to velocity, particle vorticity and leaping movement. They compared their findings with those