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Effects of surface wettability, roughness and moving wall velocity on the Couette flow in nano-channel using multi-scale hybrid method

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ABSTRACT

The present study investigated the Couette flow in a nano-channel using the hybrid method that combines the numerical solutions from the continuum region and the particle region. The governing equations in the continuum region were numerically solved using the finite volume method, while those in the particle region were numerically solved using a molecular dynamics simulation. An overlap region was defined to couple the continuum region with the particle region and to transfer the computational results obtained in one region to another region as boundary conditions. This study considered the effects of the wettability between the liquid and solid, the height of the pillar on the bottom wall, the velocity of the moving wall, and the channel height on the Couette flow in a nano-channel. The slip velocity on the wall decreases with increasing wettability because of the increasing attractive force between the fluid and solid wall. The slip velocity decreases with increasing pillar height as a result of increasing resistance to the fluid motion in the presence of pillar. The no-slip and locking conditions are independent of the moving wall velocity when the attractive force is large enough to satisfy these conditions. The slip velocity decreases as the channel height increases. When the channel height is large enough, the no-slip condition assumption at macroscale is available. The relative slip velocity and slip length are presented as a function of wettability for different velocity of moving wall and pillar heights.

1. Introduction

Advances in nanotechnology can make the micro- and nanoscale products for various applications, such as micro-/nano-electro-mechanical systems (MEMS/NEMS), micro heat exchangers, carbon nanotubes (CNT), and micromixers. Due to the small scales and the high surface-area-to-volume ratio, micro- and nanoscale systems have different flow characteristics from macroscale systems. It is important to predict the flow characteristics of nanoscale products because flow characteristics significantly affect the efficiency of the products. However, there are limitations in analyzing physical phenomena in detail using an experimental method because of expensive equipment required and technical difficulty. However, as computer analysis technology advances, numerical analyses of nanoscale system are actively conducted in order to overcome the experimental limitations.

A conventional tool for solving fluid flow problem is computational fluid dynamics (CFD) based on Navier–Stokes equations for viscous flow modeling through the continuum hypothesis assumption. However, the continuum hypothesis assumption is not applicable when the system approaches the micro- and nanoscales. However, molecular dynamics simulations can be used to model nano-fluid flow problems. Therefore, molecular dynamics simulations become a necessary and useful tool to investigate the phenomena in nanoscale systems. Many researchers have investigated flow phenomena in nano-channels using molecular dynamics simulations. Thompson and Troian [1] indicated that the well-known Navier slip boundary condition can be used when the local shear rate at the fluid-solid interface is lower than the critical shear rate. Generalized boundary conditions obtained by molecular dynamics were used to relate the degree of slip to the underlying static properties and dynamic interactions of the walls and the fluid.

Zhang et al. [2] performed molecular dynamics simulations for Poiseuille flows to study the influence of the solid-fluid coupling strength, the fluid temperature, and density of the solid wall on the velocity at the fluid boundary. Large velocity slip at the fluid

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boundary was observed for weak solid-fluid coupling, high fluid temperature, and high solid wall density. Fan et al. [3] conducted non-equilibrium molecular dynamics simulations to investigate the complex liquid flow in nano-channels in two geometrically similar flow domains with different sizes. Similarity between the global flow parameters did not imply similarity between the molecular flows. Also, nano-sized vortex flow can be developed at low Reynolds numbers due to near-wall molecules with sufficiently large momentum.

Cao et al. [4,5] revealed the effects of surface roughness on the slip flow of gaseous argon in submicron platinum channels for various geometries of the surface roughness using molecular dynamics simulations. The velocity boundary conditions depended on the Knusen number and the surface roughness. The slip length of gas flow over a surface induced by the roughness was less than that predicted by the Maxwell model and showed a non-linear relationship with the Knudsen number. Noorian et al. [6] investigated the effects of cubical and spherical roughness geometry on the flow of liquid argon through nano-channels using molecular dynamics simulations. The rough surface with cubical roughness elements has a greater effect on the flow velocity than a smooth channel. The penetration depth of the density fluctuation into the main fluid was independent of the type of the roughness elements. As mentioned in the preceding paragraph, many studies were conducted to find the effect of liquid-solid interaction and surface roughness on nano-channel flow.

However, in these methods, the system size is limited to several nanometers, because the computational cost is high when calculating the nano-channel flow using molecular dynamics simulations. Thus, in this study, a multi-scale hybrid method is adopted. This computational method couples the molecular dynamics simulations with CFD. O'Connell and Thompson [7] developed the hybrid method to combine the advantages and compensate for the disadvantages of molecular dynamics simulations and CFD. Molecular dynamics simulations have high accuracy but also high computational cost, while CFD has lower computational cost, but the continuum hypothesis assumption breaks down near the system boundary. Information is transferred in the overlap region, where the two methods are used simultaneously. Many researchers have used multi-scale hybrid methods to solve micro- and nanoscale problems [7–23]. The present study investigates the effects on the flow boundary of the surface wettability, the pillar height at the bottom wall, moving wall velocity, and the channel height.

2. Numerical methods

For the hybrid method, the domain is composed of three different regions as shown in Fig. 1. Near the moving wall region, the finite volume method (FVM) is implemented for the continuum region. Near the stationary wall region (the particle region), molecular dynamics simulation is used. There is an overlap region between the continuum region and particle region where the hybrid method is applied.

2.1. Molecular dynamics

The liquid and stationary wall in the particle region (P region) are simulated using molecular dynamics in three dimensions. The dimension of the P region used is 9.2 nm × 6.1 nm in the x- and y-directions, respectively. To consider the channel height effect on the fluid flow in the channel, the length in the z-direction varies in the range from 12.78 nm to 51.12 nm according to increasing channel height as shown in Table 1. Periodic boundary conditions are applied in the x- and y-directions. The 12-6 Lennard-Jones potential $\phi(r)$ is used to model the molecular interaction as shown in Eq. (1).

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

where ε and σ are the characteristic energy and characteristic length. The values for the characteristic energy and characteristic length are set as $\varepsilon = 1.65 \times 10^{-21}$ J and $\sigma = 0.341$ nm corresponding to the liquid argon. The cutoff radius is set to $r_c = 4\sigma$. The interaction between the solid and liquid is also modeled using the 12-6 Lennard-Jones potential. The characteristic energy and characteristic length between the solid and liquid are changed to $\varepsilon_{wf} = \beta\varepsilon$ and $\sigma_{wf} = \sigma$, where β is the wettability factor between the liquid and solid. In this study, β is varied from 0.01 to 10 to investigate the wettability effect. Newton's equation of motion is used to calculate the acceleration of argon atoms as shown in Eq. (2).

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = -\sum_{j\neq i} \frac{\partial \phi_{ji}}{\partial \mathbf{r}_i} \tag{2}$$

The Verlet velocity algorithm is used to integrate Newton's equations of motion with a time step of $\delta t_P = 0.0108$ps which corresponds to 0.005τ in LJ unit for liquid argon.

The density and temperature of the liquid between the walls are $\rho = 1378.37$ kg/m^3 and $T = 90$ K, respectively. The temperature of the liquid is maintained by a Langevin thermostat in the y -direction. The bottom wall consists of two layers of FCC (1 1 1) structured atoms and periodic rectangular pillars, which have the same density as that of the liquid atoms [7]. The bottom wall is modeled as a fixed body with a rigid structure, and particles at the bottom wall are fixed in their initial positions. The width of the rectangular pillar is 4.8 nm, and its center is located at the center of the stationary wall. The height of the pillar is varied from 0 to 4.3575 nm in order to investigate the pillar height effect. Molecular dynamics simulations were conducted using the large-scale atomic/molecular massively parallel simulator (LAMMPS) [23].

2.2. Finite volume method

The liquid in the continuum region (C region) was simulated using the finite volume method for two-dimensional incompressible Navier–Stokes equations. It is assumed that flow in the channel is two-dimensional since there is no change along the y -direction in the low- Reynolds- number flow. The governing equations are shown in Eqs. (3) and (4).

$$\nabla \cdot \mathbf{u} = 0 \tag{3}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u} = \frac{\mu}{\rho}\nabla^2\mathbf{u} - \frac{1}{\rho}\nabla p \tag{4}$$

where $\mathbf{u}$ is the velocity vector of the x and z components, respectively, and μ is the dynamic viscosity which is $\mu = 2.476 \times 10^{-4}$ Pa•s corresponding to liquid argon at $\rho = 1,378.37$kg/m^3 and $T =$ 90K.

The fully implicit scheme was used for the temporal integration of the governing Eqs. (3) and (4) in the continuum region. For the spatial integration in the continuum region, the convection and diffusion terms were discretized using the power-law and central difference schemes, respectively, under the staggered grid system. In this study, when the pressure gradient along the stream-wise direction was lower than 10^{-8}, the solution was considered to be converged. The SIMPLEC algorithm is used to solve the flow and pressure fields [24]. The size of the C region in the x-direction varies in the range from 21.3 to 85.2 nm and the z-direction varies in the range from 14.91 to 1039.44 nm. The domain of the C region is divided by a uniform grid with the number of meshes ranging