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Effects of density on flow in a nano channel using a molecular-continuum hybrid method

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ABSTRACT

A molecular-continuum hybrid method was developed to simulate micro- and nano-scale fluid flows that cannot be predicted using continuum fluidics. Molecular dynamics simulation was used near stationary solid surfaces, and Navier-Stokes equations were used in other regions. We carried out Couette flow simulation using this hybrid method and validated the results by comparing them with the analytical solution. We also studied the dependence of the velocity slip and slip length on the surface energy, liquid density, and roughness for a liquid channel flow with and without nano-structures on the solid surface. The behavior of the liquid near the solid wall changed with the surface energy as well as the liquid density. The variation of the velocity slip and slip length according to the surface energy also depended on the liquid density as well as the surface roughness. We compared the required computational time obtained from the molecular-continuum hybrid method with that obtained from full molecular dynamics simulation under the same computational condition, giving much shorter computational time for the case using the molecular-continuum hybrid method than that for full molecular dynamics simulation.

1. Introduction

Micro- and nanoscale products are developing rapidly, and the fluid behavior at these scales can influence the performance and efficiency of the machinery. Various physical phenomena change at different spatial and temporal scales. Computational fluid dynamics (CFD) based on the Navier-Stokes equations are applied at the macroscale based on the continuum hypothesis assumption. However, the assumption breaks down and the Navier-Stokes equations cannot be used at the micro- and nano-scale. Instead, molecular dynamics simulation (MDS) based on Newton's laws of motion is applied at these small scales. However, MDS is computationally costly. Therefore, it is necessary to use a molecular-continuum hybrid method, in which CFD is applied in the bulk region and MDS is applied in the vicinity of solid surfaces for high accuracy.

Many studies on the behavior of fluids at the micro- and nanoscale have been carried out. Thompson and Trolan [1] observed a Newtonian liquid under shear using MDS, which resulted in a general nonlinear relationship between the slip and the local shear rate at a surface. Ruijter et al. [2] studied the dynamic wetting of a droplet spreading by changing the strength of the solid-liquid interaction. Jeong et al. [3] used MDS to investigate both the static and dynamic characteristics of water droplets on fixed surfaces with nano-sized pillared structures. Cao et al. [4] carried out MDS to consider wetting and flow in nano-channels with nano-scale triangular structures. The nano-sized structures had an effect on both the boundary slip and friction of the flow.

O'Connell and Thompson [5] developed the pioneering hybrid method using a coupling scheme for momentum and applied it to unsteady shear flow between two surfaces. Nie et al. [6] showed excellent results for a sudden-start Couette flow with a modified momentum-coupling scheme. Wang and He [7] further modified the momentum coupling scheme. Yen at el. [8] used time-averaging terms instead of instant terms in their improved scheme to eliminate thermal noise. Sun et al. [9,10] used a hybrid method to investigate the scaling effect on flow and thermal boundaries in a large domain and the effect of the shape of roughening on flow, which would be difficult only using MDS. Although the effects of the surface energy and surface roughness in a nano channel have been studied by many researchers, studies related to boundaries

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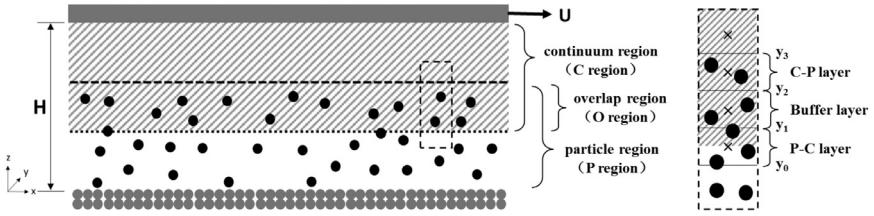

Fig. 1. Schematic of the sudden-start Couette flow with a smooth surface.

with various liquid densities in a nano channel have not been dealt with.

In this study, a molecular-continuum hybrid method is used for a Couette flow simulation in which the upper plate is moving and the lower plate is stationary. We investigated the effects of the surface energy and surface roughness on the slip at the stationary solid walls for liquid densities of $\rho = 0.7\sigma^{-3}$, $\rho = 0.81\sigma^{-3}$, and $\rho = 0.9\sigma^{-3}$. The trends of the velocity boundary condition at each density change with the various surface energies and wall roughness.

2. Numerical methodology

2.1. Domain decomposition

Fig. 1 shows the hybrid domain decomposition method. The domain has three computational regions. In the particle (P) region near the lower plate, the continuum hypothesis is not valid. Navier-Stokes equations are used in the continuum (C) region near the upper plate. In the overlap (O) region, CFD and MDS are both performed and coupled together to insure continuity between the particle region and continuum region.

2.2. Molecular dynamics simulation

In the three-dimensional MDS, the molecular interaction between Ar atoms was modeled using the shifted Lennard-Jones (L-J) potential:

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

where $\sigma = 0.341nm$ and $\varepsilon = 1.65 \times 10^{-21}J$ are characteristic length and characteristic energy of argon, respectively. The cutoff length is represented by r_C. The molecular interaction is set to zero when the atoms are separated by more than the cutoff length. The shifted Lennard-Jones potential also models the interaction between the solid and liquid atoms. The characteristic energy and characteristic length are changed to $\varepsilon_{wf} = \beta\varepsilon$ and $\sigma_{wf} = 0.91\sigma$, where β is a surface energy factor between the solid and liquid. The lower plate is set at the bottom of the particle region. The solid wall is modeled with three layers of FCC (1 1 1) structured atoms with a neighboring distance of $\sigma_W = 0.814\sigma$. This arrangement leads to a solid wall density of $\rho_W = 2.63\sigma^{-3}$, which corresponds to platinum (Pt). Newton's equation of motion is used to determine the movement of each atom:

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

The Verlet velocity algorithm is used to project the movement of the atoms at a time step of$\delta t^P = 0.005\tau$, where $\tau = \sigma(m/\varepsilon)^{1/2}$.

2.3. Finite volume method

For the continuum section, the finite volume method (FVM) based on the Navier-Stokes equations has performed in two dimensions. The governing equations the following:

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

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

where $\mathbf{u}$ is the velocity vector of the x and z components, and μ is the dynamic viscosity. The "semi-implicit method for pressure linked equations consistent" (SIMPLEC) algorithm is used to solve the two-dimensional flow and pressure fields [11]. A staggered grid is applied, which requires that the velocities u and w be located at the faces of the control volume, while the other quantities are defined at the center of the main control volumes, including pressure and density. The time step for the continuum region is determined as $\delta t^C = 50\delta t^P = 0.25\tau$. Periodic boundary conditions (PBC) are applied in the x- direction, and a no-slip boundary condition is imposed at the upper plate.

2.4. Boundary conditions

In the overlap region, the coupling scheme is executed by swapping data between the particle and continuum regions. The overlap region is divided into a P-C layer, buffer layer, and C-P layer. In the P-C layer, the molecular dynamics data is obtained by averaging particle quantities and transferring them to the continuum region as the boundary condition for the bottom of the continuum region. The coupling scheme in the P-C layer is given by Eq. (5):

$$\mathbf{u} = \left\langle\frac{1}{N^{P-C}}\sum_{j=1}^{N^{P-C}}\dot{r}_j\right\rangle_{\delta t^C} \tag{5}$$

where $\langle\rangle_{\delta t^C}$ represents the temporal averaging from $t-\delta t^C$ to t, $\dot{r}_j$ represents the velocity vector of the jth atom in the P-C layer, and N^{P-C} is the number of atoms in the P-C layer. In the C-P layer, continuum information is transferred to the particle region. The coupling scheme was proposed by Nie et al. [6] and improved by Yen et al. [8]:

$$\ddot{\mathbf{r}}_i(t) = \frac{1}{(p/2+1)\delta t^P}\left[\mathbf{u}_C\left(t+\delta t^P\right) - \left\langle\frac{1}{N^{C-P}}\sum_{j=1}^{N^{C-P}}\dot{\mathbf{r}}_j(t)\right\rangle_{p\delta t^P}\right] + \left[\frac{\mathbf{f}_i(t)}{m} - \left\langle\frac{1}{N^{C-P}}\sum_{j=1}^{N^{C-P}}\frac{\mathbf{f}_j(t)}{m}\right\rangle_{p\delta t^P}\right] \tag{6}$$

where $p = 50$, $\mathbf{u}_C(t+\delta t^P)$ is the velocity vector in the middle of the C-P layer at $t+\delta t^P$, $\langle\rangle_{p\delta t^P}$ represents the temporal averaging from $t - p\delta t^P$ to t, $\mathbf{f}_i$ and $\mathbf{f}_j$ are the interaction force acting on the ith and jth atoms in the C-P layer, and N^{C-P} is the number of atoms in the C-P layer.

To prevent the atoms from freely escaping the particle region, an external force is applied to particles in the C-P layer:

$$F_e(z) = -p_0\sigma\frac{z-z_2}{1-(z-z_2)/(z_3-z_2)} \tag{7}$$

where p_0 is the average pressure in the particle region.