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Molecular Dynamics of Fluid Properties by Spanwise Oscillations of Solid Wall

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Abstract: The fluid properties under the condition of the solid wall spanwise oscillation were studied using the molecular dynamics method. The three dimensional Couette flow model which was made up of copper wall and argon fluid was built. The fluid state of the near wall was simulated under the different oscillation parameters of solid wall and the corresponding fluid velocity field, the density distribution, the potential energy curves and the friction force were obtained. Then the influence mechanism of the wall oscillations on the frictional drag at liquid-solid interface was investigated. *The results indicate that the frictional drag between wall and fluid can be reduced effectively by applying spanwise oscillation for the solid wall* and the drag reduction rate is mainly dependent on the oscillation parameters. Meanwhile, *the decrease of fluid density near wall leads to the reduction in frictional drag at liquid-solid interface.*

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壁面展向振动流体特性的分子动力学

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摘要：应用分子动力学方法研究壁面展向振动条件下流体的流动特性。构建了由铜固体壁面与氩流体构成的三维 Couette 流动几何模型。通过对固体平板壁面施加不同振动参数的展向振动，模拟仿真了不同振动参数下近壁面流体的流动状态，得到了相应的流体流动参数，进而研究分析了壁面振动对固液界面间摩擦阻力的影响机制。研究结果表明:*对壁面施加展向振动可以有效地减小固液界面间的摩擦力*，减阻的幅度与振动参数关系很大；通过对流体的速度场及密度分布的分析，*认为固体壁面展向振动使近壁面流体密度大幅度降低是导致固液界面间摩擦力减小的主要原因。*

关键词：壁面振动；减阻；流场；分子动力学模拟

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Introduction

Human beings have been pursuing the goal of reducing the resistance of aircrafts, increasing the speed of aircrafts and saving energy. Drag reduction by wall oscillations gains more and more people's attention since Jung WJ et al.[1] found that wall spanwise oscillation could reduce drag effectively by direct numerical simulation of slot turbulence in 1992. Laadhari F et al.[2] studied the flow state of turbulence boundary layer with wall spanwise oscillation and results indicated that the smaller average velocity gradient appears on turbulence boundary layer near the oscillation wall and the

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turbulence intensity is reduced. The research has verified that wall oscillations can reduce frictional drag of the turbulence boundary layer. From then on, many scholars[3-8] also did some relevant numerical simulations and experimental researches and got same conclusions.

At present, most researches mainly concentrate on the effect of wall spanwise oscillation on fluid flow field using direct numerical simulation method based on the theory of turbulence, meanwhile, these researches are limited to high amplitude and low frequency of mechanical vibration. The supersonic vibration are not studied. Moreover, inspiring from the well drag reduction effect of the ultrasonic oscillation cutting, molecular dynamics simulation technique is adopted to investigate the influence of wall oscillations on characteristics of flow field near the wall under the wall spanwise high frequencies oscillations.

1 Simulation system

1.1 Computation model

Three dimensional Couette geometric flow model which consists of copper wall and argon fluid is built using LAMMPS[9] as shown in Fig.1. Two copper thin-walls are discretized with 5 layers of copper atoms defined by FCC lattice structure[10].

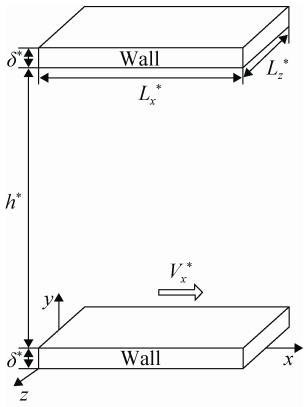

Fig.1 Molecular dynamics simulation computation model

The initial state of argon fluid also use same configuration to reduce the relaxation time and the initial density value is $\rho^* = 0.8$. The length、 width and height values of the model is L_x^*=42.7494, L_y^*=76.9489, L_z^*=34.1996 respectively. The upper and lower copper walls are identical and thickness value is $\sigma^* = 3.8475$. The total number of atoms is 91 000 with 81 000 argon fluid atoms and 5 000 copper atoms in each copper wall.

1.2 The interaction potential and parameters

In classical molecular dynamics simulations, the Lennard-Jones (LJ) method is wildly used to simulate the pairwise interaction between any two fluid monomers. The interaction between the liquid argon atoms described by this method is not only consistent with the experimental data well but simple form and less expensive calculation.

The influence of the wall oscillation on argon fluid near wall is the key attention in present work. In order to oscillate the solid wall regularly and reduce the amount of calculation, the interaction between copper atoms is overlooked and thermal freedom movement of copper atoms is restricted. The interaction defined by Lennard-Jones potential function between any two atoms except copper atoms is expressed as:

$$\varphi(r_{ij}) = \begin{cases} 4\varepsilon\left[\left(\dfrac{\sigma}{r_{ij}}\right)^{12} - \left(\dfrac{\sigma}{r_{ij}}\right)^{6}\right] & (r \leqslant r_c) \\ 0 & (r > r_c) \end{cases} \quad (1)$$

Where: σ and ε denote the length and energy scales, respectively. r is the particle spacing and r_c is the cutoff radius. In this paper, $r_c = 2.5\sigma_{\mathrm{Ar}}$ for argon atoms and $r_c = 3\sigma_{\mathrm{Ar}}$ for copper-argon atoms.

The interaction potential parameters between copper-argon atoms can be determined according to Lorentz-Berthelot principle:

$$\varepsilon_{\mathrm{Ar-Cu}}=\sqrt{\varepsilon_{\mathrm{Ar}}\cdot\varepsilon_{\mathrm{Cu}}} \quad (2)$$

$$\sigma_{\mathrm{Ar-Cu}}=\frac{1}{2}\left(\sigma_{\mathrm{Ar}}+\sigma_{\mathrm{Cu}}\right) \quad (3)$$

Where A_r and C_u are stand for argon and copper respectively.

The parameters of LJ potential function between different atoms are given in Table 1[11].

Table 1 The parameters of LJ potential between different atoms

Atom type	σ(nm)	ε(J)
Argon-Argon	0.340 5	16.5402×10^{-22}
Copper-Copper	0.233 8	65.5815×10^{-21}
Argon-Copper	0.287 2	10.4153×10^{-21}

In this simulation, the basic parameters of argon are determined as dimensionless units and expressed as: $\sigma_{\mathrm{Ar}}=0.34\mathrm{nm}$ $\varepsilon_{\mathrm{Ar}}=16.5402\times10^{-22}\mathrm{J}$ m_{Ar}=39.95×1.6747×10^{-24}g t_{Ar}=2.161×10^{-22}s for length, energy, mass, time respectively. The other physical quantities in the calculation can be transformed into dimensionless value via the above basic units. The transformation relations are given in Table 2.

Table 2 The dimensionless value transformation relation of physical quantities

Physical quantity	Transformation relation	Physical quantity	Transformation relation
Particle spacing	$r^*=\frac{r}{\sigma}$	Time	$t^*=t\sqrt{\frac{\varepsilon}{m\sigma^2}}$
Energy	$E^*=\frac{E}{\varepsilon}$	Velocity	$v^*=v\sqrt{\frac{m}{\varepsilon}}$
Force	$f^*=f\frac{\sigma}{\varepsilon}$	Temperature	$T^*=T\frac{k_b}{\varepsilon}$
Pressure	$P^*=P\frac{\sigma^3}{\varepsilon}$	Number density	$\rho^*=\rho\sigma^3$

1.3 Boundary conditions and simulation ensemble

According to the above computation model, mixed boundary conditions with periodic conditions for *x* and *z* directions and solid-wall boundary for *y* direction are adopted. The simulation system is defined in NVT ensemble and temperature around 90K is controlled using Nose-Hoover method. It is important to note that particle' velocity consists of advection velocity and thermal velocity in non-equilibrium molecular dynamics simulation. However, temperature is only closely related to thermal velocity, the advection velocity can be removed from the particle' velocity using PUT (profile-unbiased thermostat) method[12]. When calculating the temperature of the simulation system, the simulation domain is divided into several grids firstly. Then center velocity in each grid is obtained by statistic method. All atoms' thermal velocities in this grid can be achieved by removing the center velocity from each atom' s velocity. Time step is defined as $\Delta t^*=0.005$.

1.4 Wall oscillation method

The upper copper wall is fixed and the copper atoms provide constraints for the top surface of the fluid field by LJ potential energy function. In this simulation, the influence of the lower wall oscillation with different parameters on the flow field near wall are discussed. The equations of motion of upper and lower wall are given as follows, respectively:

Upper wall: $S_x^*=0, S_y^*=0, S_z^*=0$ (4)

Lower wall: $$\begin{cases} S_x^*=V_x^*t^* \\ S_y^*=0 \\ S_z^*=A^*\sin(2\pi t^*/T^*) \end{cases} \quad (5)$$

Where S_x^*, S_y^*, S_z^* are the wall displacement along *x*, *y*, *z* direction, respectively. V_x^* is the wall velocity along *x* direction, A^* and T^* are the amplitude and period of wall oscillation, respectively.

2 Simulation results and discussion

According to the simulation system and simulation steps, this paper will discuss the influence of the oscillation parameters including period (frequency) and amplitude on the fluid flow

parameters near the oscillation wall.

2.1 The influence of the oscillation parameters on the fluid flow velocity distribution

Firstly the influence of the different oscillation amplitude on the fluid velocity along *x* direction at the same period is investigated. In the present paper, the fluid field is divided into 44 layers averagely along *y* direction. The velocity component along *x* direction of all fluid atoms in each layer are recorded and then velocity of the fluid in each layer along *x* direction is achieved according to Eq.(6).

$$v_x^* = \frac{1}{N_{\text{bin}}} \sum_{\text{i}=1}^{N_{\text{bin}}} v_{ix}^* \tag{6}$$

Where N_{bin} is the total number of atoms in each layer.

The average flow velocity distributions along *x* direction within a period of time at same period (T^*=100) and different amplitude (A^*=8, 30, 80, 100) are shown in Fig.2.

As clearly observed in Fig.2, when solid wall is not overlaid with oscillation, the fluid velocity distribution along *x* direction is linear and several layers of fluid near wall have same velocity with wall approximately. While solid wall is overlaid with spanwise oscillation, the fluid velocity distributions along *x* direction become nonlinear gradually and the fluid velocity has distinct hysteresis with the increase of the amplitude.

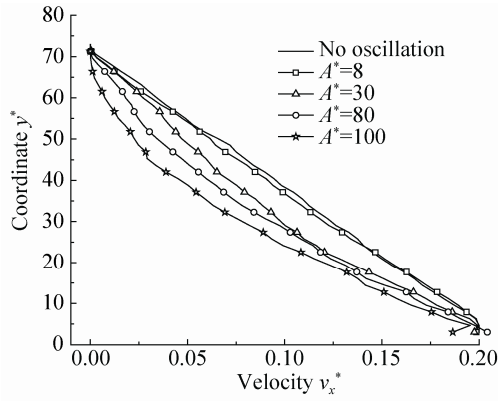

Fig.2 the influence of the oscillation amplitude on the fluid flow velocity distribution along x direction

Fig. 3 shows the influence of the spanwise oscillation period (T^*=100, 300, 500, 1000) on the fluid velocity distribution along *x* direction at the same amplitude (A^*=8). it is demonstrated that the oscillation period almost do not affect the fluid velocity distribution.

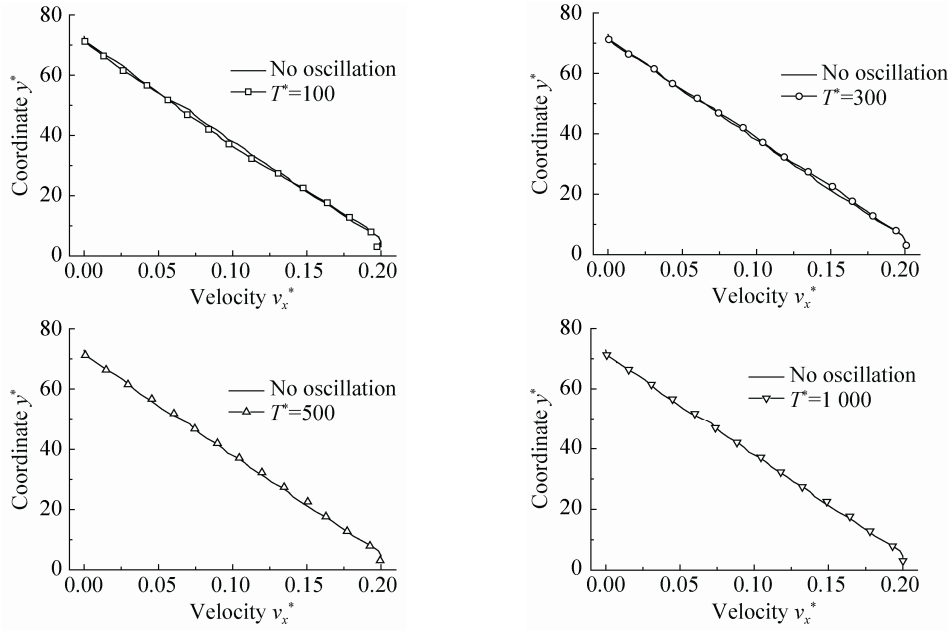

Fig.3 The influence of the oscillation period on the fluid flow velocity distribution along x direction

When solid wall is overlaid with spanwise oscillation, the wall will certainly affect the fluid velocity distribution near wall along z direction due to the effect of the copper atoms in the wall on the argon atoms in the fluid. The fluid velocity curves changing with time at y^*=6.2917 with the same oscillation period (T^*=100) and different amplitudes (A^*=8, 30, 50, 100) are shown in Fig.4.

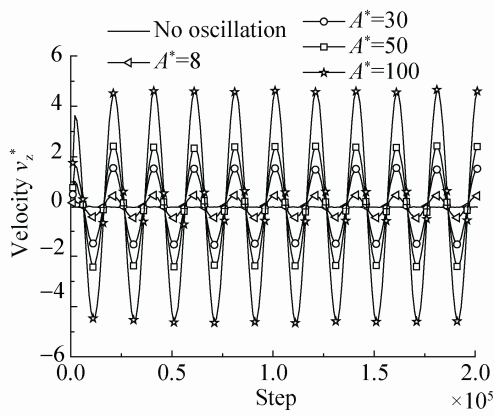

Fig.4 the flow velocity curves of the fluid layer at coordinate of y^*=6.2917 changing with the time at the different amplitude of wall

It can be seen from Fig.4, When solid wall is not overlaid with spanwise oscillation, the fluid only has thermal motion velocity component along *z* direction and its value is fixed. While solid wall is overlaid with spanwise oscillation, the solid wall will drive the fluid motion and the velocity component v_z^* curves along *z* direction are sine (cosine) curves approximately, meanwhile, the curves peak value increase with the increase of the oscillation amplitudes.

2.2 The influence of the oscillation period on the fluid density distribution

The fluid field is divided into 44 layers averagely along *y* direction, the number of fluid atoms in each layer are recorded after the simulation system reaching steady state.

The changing curves of the fluid density at the same period (T^*=100) and the different amplitudes (A^*=8,30,50,100) are depicted in Fig.5. It is shown that the flow field is described as uniform distribution except for the flow field near wall which shows the oscillation distribution without wall oscillation. It is been obviously that wall oscillation leads to the decrease of fluid density near wall after the wall is overlaid with the spanwise oscillation. With the increase of the oscillation amplitude, the degree of decrease of the fluid density is becoming distinct.

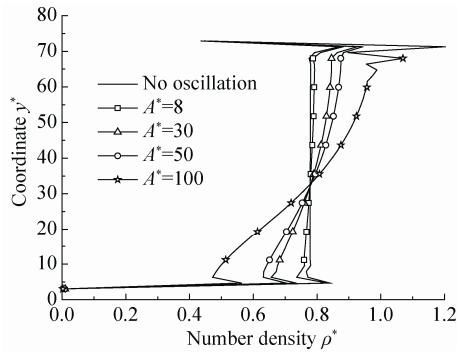

Fig.5 the influence of the oscillation amplitude on the fluid density distribution

The changing curves of the fluid density at the different periods (T^*=100, 300, 500, 1000) and the same amplitude (A^*=8) are shown in Fig.6. it is demonstrated that the oscillation period almost do not affect the fluid density distribution under the chosen parameters.

2.3 The effects of oscillation parameters on the interaction potential energy

The interaction force at the solid-liquid interface is related to the potential energy directly, so it is necessary to investigate the effects of the oscillation parameters on the interaction potential energy. Figure 7 shows the changing curves of the potential energy on the solid-liquid interface with the time at the same period (T^*=100) and different amplitudes

(A^*=8,30,50,100). After the system achieves stability, From Fig.8 it can be seen that the interaction potential energy almost do not change with time at the period (T^*=100) with lower amplitude (A^*<15), while with the increase of the oscillation amplitudes (A^*>30), the interaction potential energy changes periodically and the curves are sine (cosine) approximately. To sum up, the average potential energy at the solid-liquid interface decreases with the increase of the oscillation amplitudes.

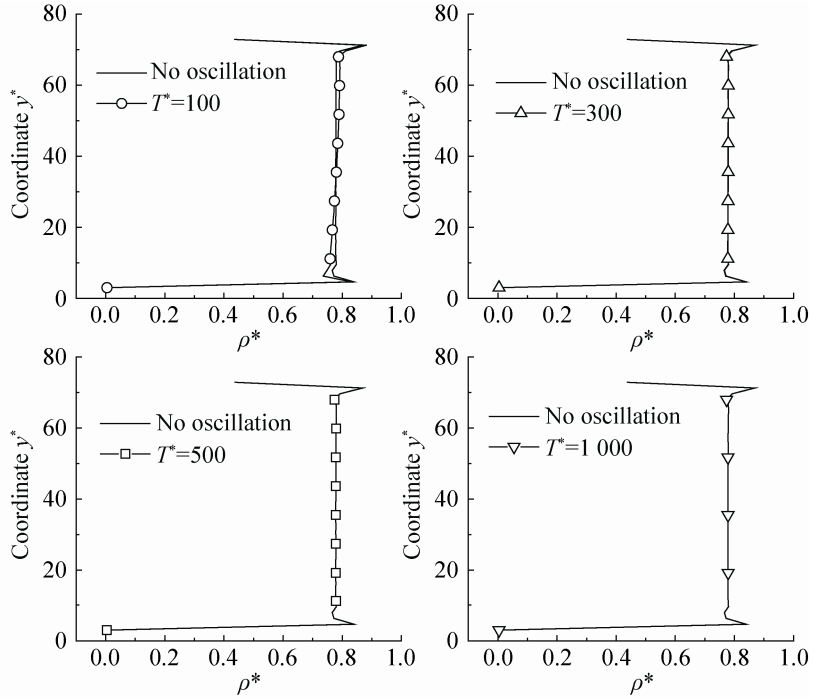

Fig.6 the influence of the oscillation period on the fluid density distribution

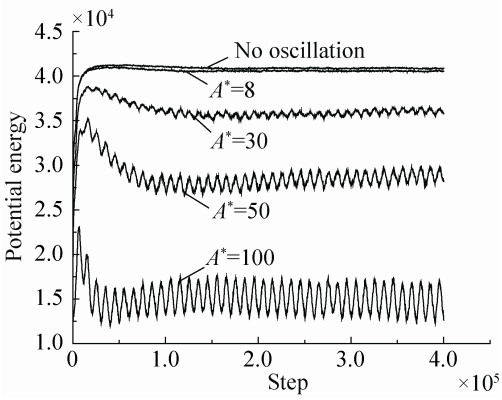

Fig.7 The effects of oscillation amplitudes on the interaction potential energy

By analyzing the change of the interaction potential energy of the solid-liquid interface at the same amplitude and different periods (T^*=100, 300, 500, 1000), it can be concluded that the potential energy is not decreased compared with no oscillation when the period have a lower value, while the larger oscillation periods has no effects on the potential energy.

2.4 The effects of oscillation parameters on the friction force at the liquid-solid interface

The friction force at the liquid-solid interface is the most important parameter in this paper, so the friction force at different oscillation parameters in each moment are recorded in the simulation. The tangential force F_x^* (or friction force) on the oscillation wall along x direction is recorded every one hundred steps. The friction represents oscillation on the microcosm, while it is obtained by statistical average of the a long period after achieving a stable state on macroscopic scale. Table3 shows the average

friction force at the same oscillation period (T^*=100) and different amplitudes (A^*=8, 30, 50, 80). It's important to note that due to the randomness of the molecular thermal movement and limit simulation time, the average friction also has certain discreteness.

Table 3 The effects of oscillation amplitude on the friction force at the liquid-solid interface

Motion situation	Lower wall tangential force F_x^*	Drag reduction rate
No oscillation	–8.602	
A^*=8	–7.7427	9.99%
A^*=30	–8.1337	5.44%
A^*=50	–8.1901	4.79%
A^*=80	–2.5443	70.42%

It can be seen from Table 3, when the wall does spanwise oscillation at a certain period and the amplitude exceeds a certain value, the friction force of the liquid-solid interface decreases sharply. There is no obvious law for the effect of oscillation parameters on the drag reduction rate under the chosen period, but the optimal oscillation parameters combination is T^*=500, A^*=50, in which the drag reduction rate reaches up to 48.78%.

Table 4 shows the average friction at the solid-liquid interface with specific amplitude (A^*=8) and different periods (T^*=100,300,500,1000). Due to the computation amount is too large, lower oscillation period is selected. From table 4 it can also be concluded that the amplitude of the drag reduction decreases with the increase of the periods under the chosen oscillation amplitude.

Table 4 The effects of oscillation period on the friction force at the liquid-solid interface

Motion situation	Lower wall tangential force F_x^*	Drag reduction rate
No oscillation	–8.602	
T^*=100	–7.742 7	9.99%
T^*=300	–8.211 3	4.54%
T^*=500	–8.219 1	4.45%
T^*=1 000	–8.233 4	4.29%

2.5 The effects mechanism of the wall oscillations on the friction force of the liquid-solid interface

(1) By analyzing the density distribution of flow field, when the wall is overlaid with spanwise period oscillations, the fluid density near wall is reduced greatly with the increase of amplitude, which leads to the decrease of fluid viscosity, so the friction force is reduced undoubtedly.

(2) By analyzing the velocity distribution of flow field, it can be concluded that the gradient of the fluid velocity along x direction near wall increases greatly with the increase of amplitude. This feature maybe increase the friction force. But the above fluid velocity is average velocity in different layers. It can be seen from Figure 4 that the fluid instantaneous velocity along z direction are positive or negative periodic oscillation. Because the fluid oscillation velocity caused by wall high frequency oscillation is larger than the average fluid velocity, meanwhile, there is a certain angle between the whole relative movement direction of the adjacent fluid layer and the flow direction, and the relative velocity vector and the direction is changing always. The effects mechanism of the fluid velocity on the friction force of the liquid-solid interface needs further research.

(3) The friction force at the liquid-solid interface is reduced with the decrease of the potential energy of interaction. Figure 7 shows that the interaction potential energy decreases with the increase of amplitude. So the decrease of interaction potential energy resulted from wall oscillation is also one of the reasons for the drag reduction.

3 Conclusions

The three dimensional couette flow model which is made up of copper wall and argon fluid is

built using LAMMPS in this paper. The state of the fluid near wall is simulated by applying spanwise oscillation with different oscillation parameters for solid wall. The corresponding fluid velocity field、the fluid density distribution、the potential energy of interaction and the friction force are investigated. The results indicate that:

(1) Wall oscillation decreases the fluid density near wall which leads to the decrease of fluid viscosity, the friction force at the liquid solid interface is reduced undoubtedly.

(2) The friction force at the liquid-solid interface is related to the potential energy. In terms of the decreases of the total potential energy by wall oscillation, the friction force at the liquid-solid interface are decreased.

(3) Wall oscillation decreases the boundary layer thickness. Meanwhile, the low fluid density and low potential energy lead to the decrease of the total potential energy and friction force.

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