Investigation on the influence mechanism of wall-fluid interaction on flow around nanoscale circular cylinder

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Abstract. The influence of atomic interaction strength between solid wall and fluid on the flow around a nanoscale circular cylinder was numerically probed with the molecular dynamics method. The results show that when the flow velocity is 2.2 and Reynolds number is 23, vortices are periodically formed behind the circular cylinder at the nanoscale, and go through the development and shedding. With the weakening of wall-fluid interaction between cylinder surface and fluid atoms, the vortex shedding period decreases, the Strouhal number increases, the weak wall-fluid interaction is beneficial for increasing vortex shedding frequency. It reveals that the length of time-averaged vortex behind the nanoscale cylinder decreases slightly with the decrease of wall-fluid interaction. Furthermore, the fluid density and velocity are symmetrically distributed along the central axis of nanoscale cylinder. As the wall-fluid interaction decreases, the binding force of cylinder surface to the fluid atoms decreases, which results in the decrease of the minimum value of fluid density in the upper right and lower right regions near the cylinder. And, the argon fluid is more prone to occur velocity slip on the cylinder surface, the corresponding velocity near the cylinder surface increases significantly.

1. Introduction

The flow of fluid through obstacles is ubiquitous phenomenon in nature, among which the square cylinder [1] and circular cylinder [2, 3] obstructed flow are the most common. Based on the experimental method [4], direct simulation Monte Carlo method [5], Lattice-Boltzmann method [6], molecular dynamics simulation [7, 8] and other methods, the disturbance characteristics of flow around the obstacles at different scales have been extensively investigated. With the development of micro/nano technology and its wide applications in thermal management of electronic devices, aerospace, thermal engineering and other fields, an enormous amount of studies focusing on the micro/nano flow [9, 10] have proved that the flow characteristics of fluid at microscope scale are different from those at conventional scale. The flow around the nanoscale circular cylinder is no exception. However, due to the limitation of experimental measurement, some potential microscopic phenomenon such as velocity slip and temperature jump can’t be well observed. Yet, studies have shown that the velocity slip has an important effect on flow and heat transfer characteristics [11, 12]. Besides, a non slip boundary condition is usually considered in traditional numerical simulation based on the continuum assumption, in which the effect of velocity slip is also ignored. Compared with the experimental research and the traditional numerical method, the molecular dynamics simulation based on the particle model would better reveal the microscope mechanism and the law of vortex shedding.
on the cylinder surface. Rapaport et al. [13] adopted the Week-Chandler-Anderson short-range potential energy model to probe the flow of fluid around the nanoscale cylinder, and obtained the characteristics of vortex generation, shedding and wake flow behind the cylinder. According to Lennard Jones (LJ) potential energy model, Sun et al. [14] studied the flow characteristics in the wake region of flow around nanoscale cylinder at different Reynolds numbers, and compared it with that of the macroscope cylinder.

Based on the above, molecular dynamics method is adopted to explore the influence mechanism of wall-fluid interaction intensity on disturbed flow characteristics of nanoscale circular cylinder. The periodical vortex generation, development and shedding are reproduced, and the characteristics of instantaneous shedding and time-averaged symmetry of flow around the cylinder are analyzed. In addition, the effects of wall-fluid interaction intensity on the vortex shedding period, the characteristics of time-averaged symmetric vortex as well as the velocity and density distribution near the cylinder are also analyzed. The microscopic mechanism of the influence of surface wettability on the disturbed flow characteristics of cylinder is investigated.

2. Physical model
The two-dimensional model of flow around the nanoscale cylinder is shown in Figure 1. At the initial stage, the argon atoms are uniformly distributed in the whole fluid calculation domain. In order to achieve physical quantities dimensionless, the LJ potential energy parameter \( \varepsilon \) and dimension parameter \( \sigma \) as well as atomic mass \( m \) of argon atom are taken as the basic units. Here, time: \( \tau^* = tf(m\sigma^2/\varepsilon)^{1/2} \), length: \( L^* = L/\sigma \), temperature: \( \theta^* = T/(\varepsilon/k_B) \), velocity: \( u^* = u/(\varepsilon/m)^{1/2} \), number density: \( \rho^* = \rho/(1/\sigma^3) \), kinematic viscosity: \( \nu^* = \nu/(\varepsilon/\sigma^2/m) \). \( k_B \) is Boltzmann constant, \( k_B = 1.38 \times 10^{-23} \) J/K. To prevent the impact of boundary on flow field, the upper and lower as well as the left and right boundaries of computational domain should be kept enough distance from the cylinder. Just as shown in Figure 1, the diameter of the platinum cylinder is \( D^* = 89.4 \), the center coordinate of the cylinder is \( 0,0 \), and the size of the simulation system is \( L_x^* \times L_y^* = 894 \times 447 \). The total number of platinum atoms is 732, the total number of argon atoms is 313788, and the fluid density is \( \rho^* = 0.8 \). The kinematic viscosity is \( \nu^* = 8.3 \) [15]. The system temperature is \( T^* = 1.0 \), the flow velocity is \( u^* = 2.2 \), Reynolds number is \( Re = 23 \). The truncation radius is 2.5 and the time step is 0.005.

![Figure 1. Configuration diagram of simulation system.](image)

3. Simulation method

3.1. Potential function
As shown in equation (1), equation (2) and equation (3), the LJ potential function [16] is adopted to characterize the interaction between fluid argon atoms, platinum cylinder atoms as well as platinum cylinder atoms and fluid argon atoms, respectively.

\[
\phi_i(r_{ij}) = 4 \varepsilon \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6}
\]  
(1)

\[
\phi_s(r_{ij}) = 4 \varepsilon \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^{6}
\]  
(2)
Here, for fluid argon atoms, \( \sigma = \sigma_A = 3.405 \text{Å}, \) \( \varepsilon = \varepsilon_A = 1.67 \times 10^{-21} \text{J}. \) For platinum cylinder atoms, \( \sigma = \sigma_P = 2.475 \text{Å} \) and \( \varepsilon = \varepsilon_P = 8.35 \times 10^{-20} \text{J}. \) In addition, the atomic mass of argon \( m = m_A = 6.63 \times 10^{-26} \text{kg}, \) and the atomic mass of platinum \( m_P = 3.24 \times 10^{-25} \text{kg}. \) For the interaction between fluid argon atoms and platinum cylinder atoms, the length scale can be given by \( \sigma_{PlAr} = (\sigma_P + \sigma_A)^{1/2} = 2.94 \text{Å} \) according to Lorentz-Berthelot rule [17]. The energy parameter \( \varepsilon_{PlAr} = \sqrt{\varepsilon_P \varepsilon_A} = 11.798 \times 10^{-21} \text{J}. \) As shown in equation (3), in order to study the influence of surface wettability on the characteristics of flow around the circular cylinder, the values of the energy parameter \( \varepsilon_{sl} \) are set as \( \varepsilon_{sl} = \varepsilon_{PlAr}. \) Here, the coefficients \( c \) are taken as 1.0, 0.1, 0.01 and 0.001, respectively, and its corresponding energy parameters of the interaction between platinum cylinder and argon fluid are \( \varepsilon_{sl} = 7.065c, \) \( \varepsilon_{sl} = 0.7065c, \) \( \varepsilon_{sl} = 0.07065c \) and \( \varepsilon_{sl} = 0.007065c. \)

3.2. Simulation details

As shown in Figure 1, the position of the cylinder remains fixed. An external force along the \( x \) direction is applied to the fluid atoms located in the inlet region with the length of 5.0. The periodic boundary condition is used in \( y \) direction. In \( x \) direction, the fluid atoms flow out from the right boundary and then in from the left boundary, but the fluid atoms coming out from the right boundary enter in the left boundary after their velocities are reassigned. To keep the system temperature constant, the velocity-scaling method is adopted to adjust the fluid temperature. The Velocity-Verlet algorithm is utilized for numerical integration. The first 2,000,000 time steps are used to achieve system relaxation. Subsequently, the next 500,000 timesteps are used for statistics of relevant parameters. Considering the characteristics and requirements of statistical physical quantities, the whole flow field is divided into 200×120 grids, and the time-averaged statistical values are obtained by using 500,000 time steps. Meanwhile, the time-averaged statistical value with less time steps (200Δτ) is assumed as the instantaneous statistical value, which is used to observe the instantaneous vortex shedding characteristics of the nanoscale cylinder.

4. Results and discussion

4.1. Instantaneous flow field distributions

Under different wall-fluid interaction, the instantaneous streamline distribution in a vortex shedding period \( \tau^* \) is shown in Figure 2, Figure 3, Figure 4 and Figure 5. As shown in these figures, (a) demonstrates that at \( \tau^*/4 \) moment, vortex V1 is generating while vortex V2 continues to develop. (b) shows that at \( \tau^*/2 \) moment, vortex V1 is developing and vortex V2 is shedding. (c) denotes that at \( 3\tau^*/4 \) moment, the vortex V1 continues to develop while the vortex V2 is emerging. (d) displays that at \( \tau^* \) moment, vortex V1 is shedding and vortex V2 is developing. The alternating generation, development and shedding of instantaneous vortices behind the cylinder are similar to the experimental results of macroscopic cylinder disturbed flow [4] at a relatively low Reynolds number, which demonstrates the reliability of the present numerical simulation method. Furthermore, the Strouhal numbers (0.145-0.203) obtained in present work are very close to that (0.2) obtained by Rapaport et al. [13]. In general, it indicates that the present numerical results are accurate and reliable.

Based on the method of collecting the instantaneous value of flow field by using the time-averaged statistical value with less molecular dynamics steps, the instantaneous vortex shedding process behind the cylinder is obtained, as well as the vortex shedding period. As illustrated in Figure 2, when the wall-fluid interaction between argon fluid atoms and platinum cylinder atoms is \( \varepsilon_{sl} = 7.065c, \) the periodic process of the two vortices is about 56,000 time steps, namely, \( \tau^* = 280. \) Thus, the Strouhal number is calculated as \( St = D/\nu \tau^* = 0.145. \)
Figure 2. Temporal streamlines in a period under the condition of \(c=1.0\).

As illustrated in Figure 3, when the coefficient is \(c=0.1\), the wall-fluid interaction between fluid argon atoms and platinum cylinder atoms is \(\varepsilon_{sl}=0.07065\varepsilon\), the periodic process of two vortices is about 51,200 time steps, the vortex shedding period is \(\tau^* = 256\) and the Strouhal number is 0.159.

Figure 3. Temporal streamlines in a period under the condition of \(c=0.1\).

As illustrated in Figure 4, when the coefficient is \(c=0.01\), the wall-fluid interaction between fluid argon atoms and platinum cylinder atoms is \(\varepsilon_{sl}=0.007065\varepsilon\), the periodic process is about 44,000 molecular dynamic steps, the vortex shedding period is \(\tau^* = 220\) and the Strouhal number is 0.185.

As illustrated in Figure 5, when the coefficient is \(c=0.001\), the wall-fluid interaction is \(\varepsilon_{sl}=0.0007065\varepsilon\), the periodic process of these two vortices is about 40,000 molecular dynamic steps, the vortex shedding period is \(\tau^* = 200\) and the Strouhal number is 0.203. Strouhal number is an important parameter to characterize the vortex shedding behind the nanoscale cylinder. The larger the Strouhal number, the shorter the shedding period and the faster the vortex shedding. Obviously, at the same Reynolds number, the vortex shedding frequency increases with the decrease of the interaction between fluid atoms and cylinder surface. It is mainly due to the less attraction of cylinder wall to fluid atoms derived from the decrease of wall-fluid interaction, which is not enough to bind the fluid atoms and make the fluid atoms escape from the cylinder surface more easily.
4.2. Time-averaged flow field distribution

Figure 6 shows the time-averaged streamlines obtained by the statistical average of 500,000 molecular dynamics steps. It is concluded that the structure of time-averaged flow field is obviously different from that of the instantaneous flow field. In the time-averaged flow field, two stable symmetric vortices are formed behind the cylinder, and there is no periodic oscillating flow in the wake region. The whole time-averaged flow field presents symmetrical distribution, which is the same as the experimental results [4] and molecular dynamics simulation results [14]. Under the different wall-fluid interactions, a stable vortex pair with the same order of magnitude as the cylinder diameter appears behind the cylinder. However, due to the variation of the wall-fluid interaction, the length of the time-averaged symmetric vortices varies to some extent.

When the potential energy adjustment coefficient $c$ varies from 1.0 to 0.001, its corresponding wall-fluid interaction are $\varepsilon_{sl}=7.065\varepsilon$, $\varepsilon_{sl}=0.7065\varepsilon$, $\varepsilon_{sl}=0.07065\varepsilon$ and $\varepsilon_{sl}=0.007065\varepsilon$, respectively, and the length of the corresponding time-averaged symmetric vortex are about $1.18D^*$, $0.786D^*$, $1.07D^*$, and $1.01D^*$. Clearly, the weakening of the wall-fluid interaction makes the length of the time-averaged symmetric vortex decrease slightly.

Figure 4. Temporal streamlines in a period under the condition of $c=0.01$.

Figure 5. Temporal streamlines in a period under the condition of $c=0.001$. 
4.3. Velocity and density distributions

The variations of fluid density at different cross sections along the flow direction are demonstrated Figure 7, where the wall-fluid interaction between argon fluid and platinum cylinder are $e_{ai}=7.065\epsilon$ and $e_{ai}=0.007065\epsilon$, respectively. The cross section at $x^*=55.875$ and $x^*=-55.875$ represents the position about 11.175 away from the nanoscale cylinder wall, and the cross section at $x^*=-2.235$ and $x^*=2.235$ represents the front and back positions of the cylinder center (about $90^\circ$), respectively. Combined with the enlarged molecular configuration of argon fluid around the platinum cylinder as shown in Figure 7 (c) and Figure 7 (d), it’s found that fluid density is uniformly distributed near the front of the cylinder ($x^*=-55.875$). As the fluid flows to the cross section of $x^*=-2.235$ and $x^*=2.235$, the fluid density near the nanoscale cylinder surface decreases, the fluid atoms become sparse in the enlarged molecular configuration shown in Figure 7 (c) and Figure 7 (d). Along the $y$ direction, the fluid density is symmetrically distributed along the central axis of nanoscale cylinder, and the farther away from the central axis, the greater the fluid density. Meanwhile, from the density distribution at the cross section of $x^*=-2.235$, $x^*=-2.235$ and $x^*=55.875$ (near the back of the nanoscale cylinder wall), it can be pointed out that the minimum density appears in the upper right and lower right regions of the nanoscale cylinder wall, rather than directly behind the nanoscale cylinder. Compared with Figure 7 (a) and Figure 7 (b), with the decrease of the wall-fluid interaction between fluid and cylinder surface, the variation trend of density in the flow field is the same, but the density near the upper right and lower right regions of the cylinder surface becomes smaller. The reason is that the decrease of the wall-fluid interaction strength weakens the binding force of platinum cylinder surface to the fluid atoms, thus further reducing the number of fluid atoms adsorbed on the nanoscale cylinder surface.
The time-averaged velocity distributions at different cross sections along the flow direction under the different wall-fluid interactions are shown in Figure 8. The velocity $u$ is symmetrically distributed in $y$ direction, and the fluid velocity near the nanoscale cylinder is smaller. At the position of $x^*=55.875$, which is in front of the cylinder, the fluid velocity is greater than zero because of no backflow. However, at the position of $x^*=55.875$, which is behind the cylinder, the fluid velocity is negative due to vortex shedding and backflow. From the velocity distributions at the cross sections of $x^*=-2.235$ and $x^*=2.235$, it’s found that the fluid velocity decreases rapidly near the cylinder surface, and the closer to the cylinder surface, the lower the fluid velocity. At the same crosssection ($x^*=2.235$), when the wall-fluid interactions are $7.065\varepsilon$ and $0.007065\varepsilon$, the corresponding fluid velocity near the cylinder surface (the first layer grid near the cylinder wall along the $y$ direction) are about 0.25 and 1.5, respectively. Obviously, the fluid velocity near the cylinder surface is greater than zero. Thus, it can be speculated that velocity slip may occur on the cylinder surface. Moreover, the smaller the wall-fluid interaction intensity, the easier the velocity slip occurs on the cylinder surface, which leads to the sharply increase of fluid velocity near the cylinder surface.

![Figure 8. Velocity distributions along y direction in different sections.](image)

5. Conclusions

In this paper, molecular dynamics simulation method is used to probe the influence of the interaction between fluid atoms and cylinder surface on the flow around the nanoscale cylinder. Similar to the flow around the cylinder at the macroscopic scale, the vortices are also periodically formed behind the cylinder at the nanoscale, and go through the development and shedding. However, the Reynolds number for periodic vortices shedding is different from that at the macroscopic scale. The conclusions are as follows:

(1) The interaction between fluid atoms and nanoscale cylinder atoms has an important effect on the vortex shedding period. With the decrease of the wall-fluid interaction, the vortex shedding period decreases and the $St$ number increases, which indicates that the weak wall-fluid interaction is conducive to increase the vortex shedding frequency.

(2) According to the results of time-averaged flow field, it’s found that although the diameter of the time-averaged vortex does not change with the weakening of the wall-fluid interaction, the length of the time-averaged vortex behind the nanoscale cylinder decreases slightly.

(3) The fluid density is symmetrically distributed along the central axis of cylinder, the farther away from the central axis, the greater the fluid density. However, the fluid density begins to decrease near the cylinder wall. The fluid density in the upper right and lower right regions near the cylinder surface is the lowest. With the decrease of the wall-fluid interaction, the number of fluid atoms adsorbed on the cylinder surface decreases, resulting in the decrease of the minimum value of fluid density near the upper right and lower right of the cylinder wall.

(4) Along the flow direction, the fluid velocity is symmetrically distributed along the central axis of nanoscale cylinder, the closer to the central axis, the lower the fluid velocity. The weakening of the wall-fluid interaction makes the binding force of the cylinder surface to fluid atoms decrease. Thus,
the fluid is more prone to occur velocity slip on the cylinder surface, which leads to the increase of corresponding fluid velocity near the cylinder surface.

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