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SIMULATION OF GAS FLOW OVER A MICRO CYLINDER

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ABSTRACT

Gas flow over a micro cylinder is simulated using both a compressible Navier-Stokes solver and a hybrid continuum /particle approach. The micro cylinder flow has low Reynolds number because of the small length scale and the low speed, which also indicates that the rarefied gas effect exists in the flow. A cylinder having a diameter of 20 microns is simulated under several flow conditions where the Reynolds number ranges from 2 to 50 and the Mach number varies from 0.1 to 0.8. It is found that the low Reynolds number flow can be compressible even when the Mach number is less than 0.3, and the drag coefficient of the cylinder increases when the Reynolds number decreases. The compressible effect will increase the pressure drag coefficient although the friction coefficient remains nearly unchanged. The rarefied gas effect will reduce both the friction and pressure drag coefficients, and the vortex in the flow may be shrunk or even disappear.

Keywords: Micro cylinder flow, Reynolds number, drag coefficient, compressible effect, rarefied effect

1. INTRODUCTION

Flow over a circular cylinder is a classical problem in fluid mechanics. The flow is usually assumed incompressible in the literature [1-5], and many flow phenomena have been observed and analyzed, especially for large Reynolds (Re) number flows. However, with the rapid progress of micro/nano-electro-mechanical systems, gas flows at the micro scale have been found exhibiting new phenomena where the incompressible flow assumption becomes invalid [6].

Micro-scale gas flow usually has small Reynolds number because of the small length scale and the low speed that is

typical for micro flows. Then the Knudsen (Kn) number becomes important because Kn is proportional to the ratio of Mach (Ma) number to Re number ($Kn \sim Ma/Re$). In fact, the Knudsen number is defined as the ratio of the molecular mean free path to the characteristic flow length, which characterizes the rarefied gas effect of the flows. Therefore, study of gas flow over a micro cylinder should consider the effects of the Reynolds number, Mach number, and Knudsen number.

In the literature, the Reynolds number effects have been most widely studied. Kaplun [1] employed matched asymptotic expansions to study the cylinder flow at very low Reynolds number where the inner and outer expansions are termed the Stokes and Oseen expansions. Tritton [2] performed a series of experiments and obtained a database of drag coefficient with the Re number ranging from 0.5 to 100. Hamielec et al. [3] and Dennis et al. [4] simulated the low Re number incompressible flow using a finite difference approach, and they investigated the drag, separation angle, and wake length in details. Recently, Sen et al. [5] used a finite element method to study the separation start Re number, separation angle, wake length and the drag. In addition, they investigated the influence of numerical setup on the simulated results such as the size of the computational domain and lateral wall boundary conditions.

The Mach number effects on the micro cylinder flows are rarely studied because these flows are often assumed incompressible due to low speed. For the rarefied gas effect, Matthews and Hill [7] investigated the drag on the nano-cylinders by using slip wall boundary conditions. They found that the slip effects could reduce the drag because the shear stress decreased due to the slip wall velocity.

In fact, general slip velocity models are derived based on one-dimensional assumption, which certainly will introduce error for two- or three-dimensional flows. In addition, slip velocity is only one indication of the rarefied gas effects on the wall surface. The constitution relation used in the Newtonian

fluid is also invalid for rarefied gas flows. Therefore, kinetic theory based is usually desired to describe micro cylinder flows.

The most widely used kinetic based simulation approach for rarefied gas flows is the direct simulation Monte Carlo (DSMC) method [8]. The DSMC method is a particle approach where a large number of particles are simulated to represent the microscopic behaviors of the real molecules. It is numerically expensive especially for low-speed flows due to the statistical scatter associated with the method. Several techniques have been developed to control the statistical scatter for very low Mach flows. One of them is the information preservation (IP) method, which was first proposed by Fan and Shen [9]. In the IP method, the information at the macroscopic level is preserved in the particles that are simulated as in the DSMC method. The preserved information is updated during the simulation and is sampled to obtain the macroscopic flow properties. Thus the statistical scatter in the IP method is small, and the method can also be applied to high-speed flows.

Furthermore, the micro cylinder flow is a multi-scale problem. The subsonic nature of the flow means that a disturbance can extend to a large distance. Then a large computational domain is generally required to implement correctly the boundary conditions. The computational domain should have at least 5 times of the cylinder diameter even with characteristic boundary conditions. For this large length scale, the continuum assumption is still valid for most of the computational domain and conventional computational fluid dynamics (CFD) techniques should be adopted to save the computational cost. Therefore, an accurate and effective way for micro cylinder flow simulation is to adopt a hybrid continuum-particle approach [10]. In the hybrid approach, a particle approach is used only for a small region around the cylinder where the kinetic effects are important, and a CFD approach is applied to the rest of the computational domain.

In this study, a hybrid continuum-particle approach is employed to simulate the micro cylinder flows with the intention to identify the rarefied gas effect and the drag force on the cylinder. A detailed description of the simulation approach is given in Section 2. The numerical results and analyses are presented in Section 3. Finally the major conclusions of the study are summarized in Section 4.

2. NUMERICAL APPROACH

We investigate the gas flows over a micro circular cylinder. The cylinder has a diameter of 20 microns and its wall temperature is assumed remaining at 273K. The free stream Mach number ranges from 0.1 to 0.8 and the flow Reynolds number based on the diameter varies from 2 to 50. As it mentioned above, such a flow is a multi-scale problem. Therefore, a hybrid continuum-particle approach [10] is adopted to simulate the flow. The coupled particle approach is the IP method and the continuum approach is a finite volume approach solving the Navier-Stokes equations.

2.1 The Information Preservation Method

The information preservation method, firstly proposed by Fan and Shen [9], is an effective particle method for simulating low-speed rarefied gas flows. The IP method was designed to reduce the statistical scatter in the DSMC method. It follows the general procedure of the DSMC method and preserves additional information at the macroscopic level in the particles and in the computational cells. In Fan and Shen's paper [9], "information velocity" is preserved in the IP method, and satisfactory results were obtained for several unidirectional, constant-density rarefied gas flows whereas the computational cost for the IP simulation was several orders of magnitude less than it required for the DSMC simulations. Later, Cai et al. [11] extended the IP method by preserving the information velocity in two components and introduced the pressure force term for 2D isothermal compressible flows. In order to simulate general low-speed gas flows, Sun and Boyd [12] proposed to additionally preserve temperature in particles, and an energy flux model and a collision model were also proposed. These schemes are designed for problems under specific conditions, and a general theoretical description of the IP method has been given by Sun and Boyd [13]. The most advanced IP scheme so far is the scheme developed by Masters and Ye [14].

For gas flow over a micro cylinder, we adopted the scheme developed by Sun and Boyd [12]. This scheme has been used to simulate the flow over a flat plate, and good results were obtained as compared with available experimental data [15]. In this scheme, the additional information preserved by every simulated particle is: information velocity $\mathbf{V}_i$ in 2D, information temperature T_i . The computational cell also preserves number density n_c , velocity $\mathbf{V}_c$ in 2D, and temperature T_c . The movement of the simulated particles follows the same procedure as in the standard DSMC method. The preserved information in particles follows these equations:

$$\frac{\partial \mathbf{V}_i}{\partial t} + \text{microscopic movement} = -\frac{1}{\rho_c} \nabla p_c + \text{collision} \quad (1)$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} V_i^2 + \frac{\xi}{2} R T_i \right) + \text{microscopic movement} = -\frac{1}{\rho_c} \nabla \cdot (\mathbf{V}_c p_c) + \text{collision} + \text{additional energy transfer} \quad (2)$$

where

$$p_c = \rho_c R T_c \quad (3)$$

$$\frac{\partial \rho_c}{\partial t} = -\nabla \cdot (\rho_c \mathbf{V}_c) \quad (4)$$

$$\mathbf{V}_c = \overline{\mathbf{V}_i} \quad (5)$$

$$T_c = \overline{T_i} \quad (6)$$

In the above expressions, $\mathbf{V}_i$ is the preserved velocity of particle i , T_i is the preserved temperature of particle i , ξ is the number of degrees of freedom of gas molecules, R is the gas constant; p_c , ρ_c , T_c are the preserved pressure, density, and temperature of the cell, respectively. The macroscopic flow field information is sampled from the information preserved in the particles [12].

The main benefit of the IP method is that it owns rather small statistical scatter as compared with the DSMC method for modeling low-speed flows, which can greatly reduce the computational cost for these flows. This feature also helps to develop an efficient adaptive hybrid scheme.

2.2 The CFD Method

The continuum approach coupled in the hybrid approach is a finite volume approach solving the Navier-Stokes equations [16]. The fluxes are evaluated with a second-order accurate modified Steger-Warming flux-vector splitting approach.

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot (\mathbf{F}_o + \mathbf{F}_\mu) = 0, \quad (7)$$

where

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ e \end{bmatrix}, \quad \mathbf{F}_o = \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u} \mathbf{u} + p \mathbf{I} \\ (e + p) \mathbf{u} \end{bmatrix}, \quad \mathbf{F}_\mu = \begin{bmatrix} 0 \\ -\boldsymbol{\tau} \\ -\boldsymbol{\tau} \cdot \mathbf{u} + q \end{bmatrix} \quad (8)$$

$$p = (\gamma - 1) \rho \varepsilon, \quad \varepsilon = e / \rho - \mathbf{u}^2 / 2 \quad (9)$$

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij}, \quad q = -\kappa \nabla \cdot \mathbf{T} \quad (10)$$

In these equations, ρ is the mass density, $\mathbf{u}$ is the velocity vector, p is the pressure, and e is the specific total energy. In order to match the variable hard sphere (VHS) [8] model used in the IP method, the viscosity coefficient μ and the coefficient of thermal conductivity κ are expressed as follows:

$$\mu = \mu_0 \left(\frac{T}{T_0} \right)^\omega, \quad \kappa = \frac{9\gamma - 5}{4\gamma - 4} R \mu, \quad (11)$$

where μ_0 is the viscosity coefficient at temperature T_0 , ω is the viscosity temperature index in the VHS molecular model, and R is the specific gas constant.

2.3 The Hybrid Continuum-Particle Approach

There are two critical issues for a hybrid scheme that two approaches are coupled to solve the flow by dividing the computational domain. One is where to place the interface for the coupled approaches, and the other is how to exchange information at the interface.

For the interface location, there are several considerations. First, both solvers must be valid to simulate the flow near the interface. This is usually evaluated using a continuum breakdown parameter. Second, the continuum domain should be as large as possible in order to achieve the maximum numerical efficiency for the hybrid approach. Third, detailed implementation of the hybrid scheme will affect the performance of the breakdown parameter. Therefore, the cutoff value of a continuum breakdown parameter is conservatively selected. In this study, the gradient-length local Knudsen number Kn_{GLL} [17] is selected as the continuum/particle interface indicator, and 0.005 is used as the cutoff value of this continuum breakdown parameter. Thus the interface location is not fixed in our scheme, and it is adaptive during the simulation.

At every time step, the continuum and IP solvers exchange information through the interface. The IP method has preserved the macroscopic information for cells that has very small statistical scatter. Then the continuum approach can directly use the macroscopic information preserved in the IP cells to evaluate the fluxes at the interface, which costs much less than that required by other hybrid approaches. On the other side, the IP solver requires the CFD part to provide boundary conditions to generate particles. For this purpose, buffer cells and reservoir cells are placed in the continuum domain along the interface. Particles are simulated in the buffer cells and reservoir cells, thus it is avoided to directly generate particles through the interface. This technique has been proved to be effective and stable, which is also adopted by others [18]. Detailed implementation of the scheme is referred to reference [10].

3. RESULTS AND DISCUSSION

The CFD solver and the hybrid approach introduced are used to study the flow over a micro cylinder whose diameter is 20 microns. The temperature of the cylinder is fixed at 273K during the simulation and full momentum and thermal accommodation is assumed. The free stream is air with a temperature of 273K. The flow condition is specified by the Mach number and the Reynolds number. The Mach number is defined as

$$Ma = u_\infty / \sqrt{\gamma R T_\infty} \quad (12)$$

and the Reynolds number is defined as

$$Re = \rho_\infty u_\infty D / \mu_\infty \quad (13)$$

where γ is the ratio of specific heats and D is the diameter of the cylinder. The Knudsen number is not an independent variable and is related to the Mach and Reynolds numbers as

$$Kn = 1.19 Ma / Re \quad (14)$$

A typical computational domain is shown in Fig. 1, where only half of the cylinder is simulated because of its geometric symmetry. The inflow and outflow boundaries are implemented using the characteristic boundary conditions [19]. The effect of the domain size on the drag is investigated with a case having the Reynolds number of 10 and Mach number of 0.2. Figure 2 shows the drag coefficient predicted using the CFD solver. Clearly, the size of the computational domain will affect the results. It seems that when the domain radius is 20 times of the cylinder diameter, the error of the predicted drag is within 1.5%. In this study, we fix the computational domain with its radius at

FIGURE 1. Illustration of the computational mesh (300×180).

FIGURE 2. Drag coefficient predicted using the CFD solver by varying the computational domain for the case: $Re=10$, $Ma=0.2$.

FIGURE 3. The schematic figure of local computational mesh and the continuum/particle interface (dashed line).

20 times of the cylinder diameter and the cells are clustered to the cylinder. When the hybrid approach is employed, a typical continuum-particle interface is illustrated in Fig. 3 where the region near the cylinder is the particle domain and the cell size in this domain is less than the local molecular mean free path.

3.1 Effects of the Reynolds Number

The Reynolds number is the key dimensionless parameter for incompressible flows. We use the CFD solver to study the effects of the Reynolds number by fixing the Mach number at 0.2, which is generally regarded as incompressible when the Mach number is less than 0.3. Figure 4 shows the density field and streamlines for the cases when the Reynolds number is between 2 and 50. The streamline patterns agree well with those in the literature [3-5]. Specifically, there is no separation when the Reynolds number is below 5 (no agreement has been reached on the exact value of the laminar separation Re yet); and once the separation happens, the length of the wake (vortex) grows approximately linearly with the Reynolds number.

A careful examination on the density contours reveals an interesting phenomenon. The density could have obvious variation at low Reynolds number flows as shown in Fig. 4. Specifically, the compressibility of the flow increases when the Reynolds number decreases. For instance, the density (dimensionless) at the stagnant point should be around 1.02 if the isentropic assumption is followed. From Fig. 4, the stagnant density is close to 1.03 at $Re=50$, and it increases to 1.06 when

$Re=2$. This is mainly because the viscous effects are neglected when the isentropic assumption is used.

It can be derived from the steady continuity and momentum equation that the stagnant density is a function of the Reynolds number as well as the Mach number:

$$\frac{\rho_0}{\rho_\infty} = F\left(Ma, \frac{Ma^2}{Re}\right) \quad (15)$$

where, ρ_0 and ρ_∞ is the stagnant and far field density respectively. Because the second variable depends also on the Reynolds number, its value increases when Re decreases. Therefore, it is necessary to consider compressible effects for low Reynolds number flows even when the Mach number is small.

FIGURE 4. Density contours and streamlines simulated using the CFD method at $Ma=0.2$. (a) $Re=2$; (b) $Re=5$; (c) $Re=10$; (d) $Re=20$; (e) $Re=50$.

FIGURE 5. Effects of the Mach number on the flow field: pressure contours and streamlines. Left side: $Re=2$, right side: $Re=50$

3.2 Effects of the Mach Number

Figure 4 has shown that the low Reynolds number gas flows may be compressible. In this section, we investigate the Mach number effects on the flows at different Reynolds numbers.

Figure 5 shows the pressure contours and streamlines at several Mach numbers when the Reynolds number is 2 and 50, respectively. In the figure, the pressure is normalized as pressure coefficient so that the difference in contour profiles can be well identified at different Mach and Reynolds numbers. As shown in the figure, the structure of the pressure contours and streamlines looks very similar regardless of the Mach number. There are some slight differences though. For instance, the high-pressure region increases with the Mach number when $Re=50$.

The Mach number effects on the streamlines are also not obvious, which is different from the Reynolds number. Careful inspection shows that the streamlines are slightly pushed outward from the cylinder as the Mach number increases. For the case with $Re=50$, the length of the separation vortex, an important parameter of the flow over a cylinder, increases with the Mach number.

In summary, the Mach number has little effects on the flow structures except some minor effects on detailed structure.

3.3 Rarefied gas effect

The Knudsen number is directly related to the Mach and Reynolds numbers, which is not an independent variable. The

FIGURE 6. Rarefied gas effect: pressure contour and streamlines, comparison between the CFD and Hybrid results at $Re=10$; (a) $Ma=0.1$, (b) $Ma=0.2$, (c) $Ma=0.4$.

Knudsen number effects, however, can be analyzed by comparing the compressible CFD and kinetic hybrid results for a flow at the same Mach and Reynolds numbers. This is because the CFD results do not contain rarefied gas effect and the hybrid approach can capture these effects. Therefore, the difference between the two results reflects the rarefied gas effect of the flow.

Figure 6 compares the pressure contours and the streamlines predicted using the CFD and hybrid approaches for the case when $Re=10$ and $Ma=0.1, 0.2, 0.4$, respectively. It seems that the rarefied gas effect has little influence on the pressure field since the pressure does not have much change even when the Knudsen number is about 0.05 ($Ma=0.4$). This can also be seen from the surface pressure as shown in Fig. 7. The streamlines, however, have obvious change when the

Knudsen number increases. When the Knudsen number is 0.012 ($Ma=0.1$), the vortex predicted by the hybrid approach is similar to the one obtained using the CFD solver. Then when the Knudsen number increases, the size of the vortex predicted by the hybrid approach decreases and the vortex disappears when the Knudsen number is about 0.05. This means that the rarefied gas effect smoothes the flow field. In fact, the adverse pressure gradient at the surface remains for high Kn flows, the disappearance of the vortex is mainly due to the slip velocity. Figure 8 shows the slip velocity for the case with $Re=10$. The slip velocity increases when the Knudsen (or Mach) number increases, which is the reason that the rarefied flow has strong ability to overcome the adverse pressure gradient, and thus the separation of the flow is delayed or even does not appear. It is a widely accepted fact that the slip velocity depends on the flow Knudsen number. However, Fig. 8 (b) shows that the slip velocity also depends on the Reynolds or Mach number. At the same Knudsen number, the slip velocity (dimensionless) increases with the Reynolds (or Mach) number. It is also noticed that the slip velocity is rather large, which may indicate that the local characteristic length of the flow is small.

3.4 Drag on the Cylinder

Drag on the cylinder is probably the most interested quantity for flow over the cylinder. From the simulated surface pressure and shear stress, we can obtain the drag coefficient on the cylinder from both the CFD and hybrid results. The drag coefficient is defined as follows:

$$C_D = \frac{F_D}{0.5 \rho_\infty U_\infty^2 D} \quad (16)$$

where, F_D is the force on the entire cylinder.

FIGURE 7. Comparison of pressure coefficient on the cylinder

surface between CFD and hybrid results (Re=10).

FIGURE 8. Slip velocity at different Kn numbers: (a) at the same Re number; (b) at different Re number

FIGURE 9. Drag characteristics: C_D (total drag coefficient); C_{Dp} (pressure drag coefficient); C_{Df} (frictional drag coefficient)

Similarly, the pressure drag coefficient is defined as C_{Dp} where the force is the pressure force and the friction drag coefficient is defined as C_{Df} where the force is the friction force.

Figure 9 shows the drag coefficient at several flow conditions predicted by both the CFD and hybrid approaches. It is clear that the compressible effect on the flow will increase the

FIGURE 10. Drag coefficient calculated by the Hybrid and CFD method when $Ma=0.1$, and compared with theoretical, experimental and numerical results in the literature

drag coefficient on the cylinder as shown in Fig. 9a. This increase mainly comes from the pressure drag coefficient (Fig. 9c) because the Mach number can significantly change the pressure distribution on the cylinder surface (Fig. 7a). The Mach number can also affect the friction drag coefficient. However, the increase of the friction drag coefficient (Fig. 9e) is rather small as compared with the pressure drag coefficient when increasing the Mach number.

When the rarefied gas effect is included, the hybrid results are shown in Fig. 9(b, d, f). Some data for high Knudsen number flows ($Kn \sim Ma/Re$) are not shown because a steady state is not achieved for those cases partially because of the particle fluctuations. By comparing Fig. 9c and Fig. 9d, it is reasoned that the rarefied gas effect can reduce the pressure drag coefficient on the cylinder, since the pressure drag coefficient increases with the Mach number in the CFD results whereas it decreases with the Mach number in the hybrid results for small Reynolds number (large Knudsen number) flows. The rarefied gas effect also applies to the friction drag coefficient. Because the slip velocity on the cylinder surface increases with the Knudsen number, the shear stress or the gradient of the parallel velocity is decreased when the rarefied gas effect is involved. Because the compressibility has little effect on the friction drag, the decreasing of the friction drag coefficient with an increasing Mach number is attributed to the rarefied gas effect. The total drag coefficient on the cylinder is then reduced when the rarefied gas effect is included. Since the compressible effect will increase the drag coefficient on the cylinder, the rarefied gas effect and the compressible effect will compete on the drag coefficient when the Mach number changes. It is found (Fig. 9b) that the compressible effect is the dominant effect when $Re > 10$ whereas the rarefied gas effect is stronger than the compressibility effect when $Re < 10$.

Comparison is also made between the present results and those from the literature. Figure 10 shows the incompressible data from several references and the present CFD and hybrid

results when $Ma=0.1$. Very good agreement is achieved among all the plotted data when $Re > 10$. However, there is difference when $Re < 10$ and the difference increases as the Reynolds number gets small. The difference may come from the physical geometric setup or the domain setup in the computation, which may need further study.

4. CONCLUSION

Gas flow over a micro cylinder has been numerically simulated using both a continuum NS solver and a hybrid continuum-particle approach. Several interesting phenomena have been observed for the studied compressible low Reynolds number flows.

First, the compressibility of flows increases when the Reynolds number decreases. The density variation is much larger than that allowed by the isentropic assumption when the Reynolds number is less than 10. Gas flows at the micro scale is usually compressible even at low Mach number.

Second, the Mach number affects the flow field and thus the drag coefficient of the cylinder depends on the Mach number. High Mach number flows have strong pressure variation (non-dimensionalized) and large drag coefficient. In addition, if there is flow separation, the length of the separation vortex will increase when the Mach number increases.

Third, the rarefied gas effect is important for low Reynolds number gas flows. The slip velocity is obvious for the micro scale flows, which could delay or even get rid of the flow separation. Both the friction and pressure drag coefficients are reduced when the rarefied gas effect is considered.

Finally, the drag coefficient of cylinder increases when the Reynolds number decreases. The compressible effect will increase the drag coefficient whereas the rarefied gas effect reduces the drag coefficient. It turns out that the drag coefficient increases with the Mach number at large Reynolds number ($Re > 10$) whereas it decreases with the Mach number for low Reynolds number flows.

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