Particle Flows around an Intruder

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Introduction.— To know the fluid flows around an intruder depending on the Reynolds number is a fundamental problem [1, 2]. When the flow speed is low, the drag force acting on a spherical intruder obeys Stokes’ law in which the drag is proportional to the speed, the viscosity of the fluid, and the radius of the intruder. Whereas the drag force satisfies Newton’s law in the high Reynolds number, in which the drag is proportional to the square of the moving speed and the cross section.

We believe that the drag force still satisfies Stokes’ law even for low speed molecules [3–7]. It is known that Stokes’ law can be used only for systems in the zero Knudsen number limit, the ratio of the mean free path to the intruder size [8–12]. The correction to Stokes’ drag for rarefied gases in the low Knudsen number is theoretically confirmed by the kinetic theory [8–12]. Whereas the drag force acting on slowly moving intruders in the large Knudsen number satisfies Epstein’s law [13–15]. It is known that the drag law depends on the distance from the boundary of a container of particles through the simulation [3] and the theory of the fluid mechanics [16]. We also note that the Kármán vortices have already been observed in molecular dynamics (MD) simulations [3, 17].

There are various experimental and numerical studies on the drag forces acting on an intruder in granular flows [18–31]. Variety of velocity dependences of the drag forces acting on an intruder in granular experiments and simulations. The granular jet experiments [18–31] and simulations [32–35] suggest that the granular jet flows can be approximated by a perfect fluid model [33, 34].

In this Letter, we numerically study the drag force acting on a spherical intruder in particle flows by controlling the ratio of the injected speed of the particles to the thermal speed which is proportional to the sound speed in terms of the MD. We characterize the turbulent-like behavior of particle flows behind the intruder with the aid of the second invariant of the velocity gradient tensor and the relative mean square displacement for large speed regime. We also characterize the scattering of particles by the intruder using the angular distribution function of scattered particles.

| $D_c/d$ | $N_s$ | $N$ | $R/d$ |
|-------|-------|-----|-------|
| 5     | 144   | 30000 | 10    |
| 13    | 744   | 101250 | 10    |
| 28    | 3365  | 810000 | 30    |

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When the mobile particles collide with the intruder, the particles reflect at random with the temperature \( T \), where we set \( T_w = T \) for simplicity. We examine two cases for the systems behind the intruder: one is a free scattering case, and another is a confined case, where the scattered particles are still confined in the tube. The used parameters are listed in Table I.

In the following, all quantities with the superscript * represents the quantities nondimensionalized by \( m, d, \) and \( k \). We use the time-averaged drag force in a steady state, and fix the speed \( V^* = 0.1 \). We have verified that the results of our simulation for \( V^* = 0.1 \) are consistent with those of the hard-core particles.

\[ D = \frac{\pi}{3} nm(D + d)^2 v_T V, \]

which agrees well with the simulation results for \( V \lesssim v_T \) as shown in Fig. 2.

Let us characterize the particle flows behind the intruder for large \( V \). We introduce the second invariant of the velocity gradient tensor \( Q = (1/2)(-S_{ij}, S_{ij} + W_{ij} W_{ij}) \) where \( S_{ij} = (1/2)(\partial_i u_j + \partial_j u_i) \) and \( W_{ij} = (1/2)(\partial_i u_j - \partial_j u_i) \) \[ 37 \]. Here, we adopt Einstein's rule for \( i \) and \( j \) where duplicated indices take summation over \( x, y, \) and \( z \). Figure 5 shows the contour of \( Q = 0 \), where the field is coarse-grained with the scale \( w = 2D \) for visibility \[ 38 \]. The vortex rich regions \( Q > 0 \) emerge behind the intruder. This behavior is similar to that observed in turbulent flows induced by an intruder.

Let us study how the particles are scattered after collisions with the intruder. We only focus on the relative motion of the particles which collide with the intruder almost simultaneously through the mean square displace-
FIG. 4. (a) The time evolution of the density profile at $t^* = 0$ (red solid line), 10 (blue dashed line), and 30 (black dotted line). The arrow indicates the direction of the diffusive front. (b) The expansion wave ($\phi = 0.15$) for $V/v_T = 1.0 \times 10^{-1}$ (open circles) and $1.0 \times 10^{-0.5}$ (open squares). The corresponding solid lines represent the expansion speeds $V_p$.

FIG. 5. Contour plot of the second invariant $Q = 0$ for $\phi = 0.40$, $D = 7d$, and $V/v_T = 10$. The arrow indicates the flow direction.

FIG. 6. The mean square displacement between two particles for $V/v_T = 1.0 \times 10^{3}$ (solid line) and $1.0 \times 10^{1}$ (open circles). The dotted line shows the exponent 2.2.

moment

$$\Delta(t) \equiv \langle |\delta \mathbf{r}_i(t) - \delta \mathbf{r}_j(t)|^2 \rangle / d^2,$$

with $\delta \mathbf{r}_i(t) = \mathbf{r}_i(t + t_c) - \mathbf{r}_i(t_c)$, where we only select two particles ($i$ and $j$) within the interval $|t_i - t_j| < \Delta t_{th} \equiv 10 \sqrt{m/k}$ with the collision times $t_i$ and $t_j$ with the intruder for $i$-th and $j$-th particles, respectively. Note that $t_c$ in Eq. (3) is larger time of $t_i$ and $t_j$. Figure 6 shows the super-ballistic behavior $\Delta(t) \sim t^{2.2}$. This behavior is analogous to the relative motion of two tracer particles in turbulent flows, which is known as Richardson’s law $\Delta(t) \sim t^3$ [39-41]. We have checked that this result is insensitive to the choice of $\Delta t_{th}$ in the range $\sqrt{m/k} \lesssim \Delta t_{th} \lesssim 20 \sqrt{m/k}$. The exponent 2.2 for the super-ballistic $\Delta(t)$ in our system seems to be much smaller than 3 for $\Delta(t)$ in turbulent flows. This is because the fluid flow behind the intruder in our system is not a fully developed turbulence but is a weak turbulence.

Next, we consider the scattering angle distribution of the mobile particles. The azimuthal angle is stored when the particles reach the region $|r_i| = 15d$. The behavior of the angular distribution $\rho(\theta)$ for $V/v_T \gtrsim 1$ completely differs from that for $V/v_T \lesssim 1$ as shown in Fig. 7.

For $V/v_T \gg 1$, the angular distribution of scattered particles has a sharp peak around the opening angle, which is the half of the apex angle of the cone of the beam scattered after collisions with the intruder [32, 33] as shown in Fig. 8. We also note that this opening angle can be explained by a phenomenology as in Ref. [32]. Because we use repulsive and elastic particles, the opening angle is expressed as

$$\theta_0 = \cos^{-1} \left[ 1 - \left( \frac{D}{2R} \right)^2 \right],$$

with

$$\Delta(t) \equiv \langle |\delta \mathbf{r}_i(t) - \delta \mathbf{r}_j(t)|^2 \rangle / d^2,$$
for $D < 2R$ [32]. When we substitute $D = 7d$ and $R = 10d$ into Eq. (1), we obtain $\theta_0 = 0.50$ (rad), which roughly agrees with the simulation results (see Fig. 7). For $V/v_T \ll 1$, on the other hand, the particles are scattered in various direction as shown in Fig. 7.

Discussion.— In our setup, we have not observed Stokes’ flow around the intruder. This is because the mobile particles are packed in the tube as an initial condition. As already explained, the expansion wave exists and the drag force acting on the intruder, known as Epstein’s law, is determined from this wave. To realize Stokes’ flow, we should simulate the situation for $V/v_T \ll 1$ [33].

Conclusion.— We have numerically investigated the particle flows injected as a beam and scattered by a spherical intruder. We found the crossover from Epstein’s law to Newton’s law, depending on the ratio of the speed to the thermal velocity, which can be explained by a simple collision model. The turbulent-like behavior has been also observed, where the mean square displacement is super-ballistic. The scattering of particles by the intruder is also characterized by the angular distribution function of scattered particles.

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Supplemental Materials: Particle Flows around an Intruder

Effect of the geometry of the intruder

In this section, let us check the dependence of the boundary condition between the intruder and the mobile particles. Here, we refer the intruder introduced in the main text as “thermal and bumpy”, because the mobile particles reflect at random when they collide with the intruder, and the small particles are attached on the surface of the core particle. We prepare three different types of the intruders: (i) “reflective and smooth,” (ii) “reflective and bumpy,” and (iii) “thermal and smooth.” The first intruder consists of only one core particle, and the reflection between the intruder and the mobile particles is elastic. The second one consists of the core particle and the small particles on its surface, where we have used the boundary condition as that used in the first case. The third one consists of only one core intruder, where we have used the thermal boundary condition as used in the main text. Figure S1 plots the results of the drag forces under various boundary conditions. The results clearly indicate that the boundary condition on the intruder is not important for the drag force. This is because the force acting on the intruder is almost determined from the region in front of the intruder as explained in the main text.

![Figure S1](image)

FIG. S1. Plots of the drag force against the scaled collision speed $V/v_T$ for free scattering case with $\phi = 0.40$ and $D = 7d$.

Vorticity

In this section, we plot the vorticity induced by the scattering of the intruder. In the following, we convert the Cartesian coordinate $(x, y, z)$ into the cylindrical coordinate $(r, \varphi, z)$, in which the common $z$-axis is parallel to the flow direction. Here, the velocity components in the cylindrical coordinate $(v_r, v_\varphi)$ are expressed as

$$\begin{align*}
v_r &= v_x \cos \theta + v_y \sin \theta \\
v_\varphi &= -v_x \sin \theta + v_y \cos \theta \quad ,
\end{align*} \quad (S1)$$

where $(v_x, v_y)$ are the velocity components represented by the Cartesian coordinate. Because the twisted structure of the flow field is not observed in our simulation, we focus on the flow structure in $rz$-plane. Let us introduce the vorticity in $rz$-plane as

$$\omega_{rz} = \frac{\partial v_z}{\partial r} - \frac{\partial v_r}{\partial z} \quad (S2)$$

Figure S2 shows a typical snapshot of the vorticity field in $rz$-plane. The positive vorticity regimes are generated in the vicinity of the intruder and move toward the downstream. Here, the positive vortex corresponds to the flow rotating counterclockwise near the intruder. (See the movie in the Supplemental Material S1.)
FIG. S2. Vorticity field behind the intruder for $V/v_T = 10$. The color represents the value of $\omega_{rz}/\omega_{\text{max}}$ with $\omega_{\text{max}} = 5.0 \times 10^{-3}(k/m)^{1/2}$. The arrow indicates the flow direction.

**Legendre coefficients**

In this section, we analyze the angular distribution in terms of the Legendre polynomials as

$$\rho(\theta) = \sum_{\ell=0}^{\infty} A_\ell P_\ell(\cos \theta),$$  \hspace{1cm} (S3)

where $P_\ell(x)$ is the Legendre polynomial of degree $\ell$ \[S2\], and $A_\ell$ is the coefficient defined by

$$A_\ell = \frac{2\ell + 1}{2} \int_{-1}^{1} \rho(\theta) P_\ell(\cos \theta) d\cos \theta.$$  \hspace{1cm} (S4)

Figure S3 shows the coefficient for each degree $\ell$. The coefficients converge slowly to zero for large $\ell$. For $V/v_T \gg 1$, $A_\ell$ has a peak at $\ell = 2$.

![Legendre expansion graph](image)

**Volume fraction dependence of the sound speed**

In this section, we show how the sound speed depends on the volume fraction. Because the volume fraction of the mobile particles is finite, the equation of state deviates from that for the ideal gas. Thus, the equation of state at finite density is fitted by the Carnahan-Starling equation \[S3\]

$$\frac{p}{nT} = Z(\phi) = \frac{1 + \phi + \phi^2 - \phi^3}{(1 - \phi)^3},$$  \hspace{1cm} (S5)
where $p$ is the static pressure. For the adiabatic process, the first law of thermodynamics becomes

$$C_v dT + T \left( \frac{\partial p}{\partial T} \right)_V \frac{dL^3}{N} = 0,$$

(S6)

where $L^3$ is the volume, $C_V = 3/2$ is the heat capacity at constant volume. Substituting the equation of state (S5), the following quantity is conserved:

$$\log \frac{p}{\phi Z(\phi)} - \frac{2}{3} \int_\phi ^{\phi^{-1}} Z(\phi')d\phi' = \text{const}.$$

(S7)

Then, the sound speed in the adiabatic process is given by

$$c(\phi) = \sqrt{\left( \frac{\partial p}{\partial \rho} \right)_S} = f(\phi) \sqrt{\frac{T}{m}},$$

(S8)

with

$$f(\phi) = \sqrt{\frac{5 + 10\phi - 3\phi^2 - 24\phi^4 + 37\phi^6 - 22\phi^7 + 5\phi^8}{3(1 - \phi)^6}}.$$ 

(S9)

Figure S4 shows the volume fraction dependence of the coefficient $f(\phi)$. When we use the expansion speed $V_p' = \sqrt{c(\phi)V}$, the drag force for the low $V/c$ cannot be captured as shown in Fig. S5.

![Graph](image)

**FIG. S4.** Plot of $f(\phi)$ as a function of the volume fraction. The dashed line shows $\sqrt{5/3}$, which is the coefficient for the ideal gas.

[S1] See the ancillary file for the movie for $V/v_T = 1.0 \times 10^3$.
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FIG. S5. Plots of the drag force against the dimensionless velocity characterized by the sound speed for free scattering and confined cases for various $\phi$ and intruder sizes $D$. The dashed and dotted lines represent the collision model \(^{(1)}\) and \(^{(2)}\) with the expansion speed $\sqrt{c(\phi)V}$, respectively.