A fully resolved smoothed particle hydrodynamics-discrete element method study of the rheology of suspensions: The role of inertia and grain shape

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ABSTRACT
This paper presents a numerical study on suspensions of monodisperse non-Brownian grains in a Couette flow. The fully resolved coupled smoothed particle hydrodynamics and discrete element method is employed to model the motion of arbitrarily shaped grains in a viscous fluid. The numerical method is benchmarked against its capability in accurately handling grain–fluid hydrodynamics and inter-grain collisions. It is then used to simulate suspension flows of varying particle Reynolds and Bagnold numbers subjected to different shear rates, solid concentrations, and solid-to-fluid density ratios. A special focus is placed on the effect of grain shape with different aspect ratios and convexities on the flow behavior. Both the inertia and the grain shape are found to affect the grain–fluid and inter-grain interactions and uniquely contribute to the overall shear stress and the rheology of the suspension. The local profiles of solid concentration suggest the presence of grain layering near the boundary walls, which becomes more pronounced with higher solid concentration and inertia, and increased non-circularity in grain shape. A further examination of the pair distribution function and average particle rotation reveals a strong correlation between suspension viscosity and grain microstructure and kinematics.

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I. INTRODUCTION
Suspensions of solid grains in a fluid are prevalent in industrial processes, including paints, food processing, waste disposal, and fresh concrete, and present in natural occurring processes such as lavas, mudflows, and gravity currents. The interactions between solid grains and fluids are frequently diverse and complex, involving visous shear, turbulence, solid–fluid hydrodynamics, and inter-grain contacts. Indeed, suspension flows remain one of the challenging flow patterns that are not fully understood.

Dimensionless numbers have been defined to characterize the flow regime of non-Brownian suspensions. Popular ones include the particle Reynolds number \( R_e \) and the Bagnold number \( B_o \). Most existing numerical studies on suspensions have focused on the limiting case at vanishing Reynolds number using algorithms such as Stokesian dynamics. Key findings from these studies include the microstructural anisotropy of grain pair distribution. It is supposed to be a major contributor to the non-Newtonian behavior of suspensions, often resulting in shear-thickening.

Among recent advancements in numerical methods, direct numerical simulation (DNS) has become prevailing for simulating suspensions, e.g., using the Lattice-Boltzmann method (LBM), immersed boundary method (IBM), and the fictitious domain method (FDM). These methods are suitable for analyzing inertial flows, arbitrarily shaped grains, and non-Newtonian fluids. Focusing on the weak inertia case, Patankar and Hu investigated the effect of finite \( R_e \) on the rheology of a dilute suspension of neutrally buoyant circular grains and attributed shear-thickening to the slower normalized angular velocity of grains as the Reynolds number increases. Kulkarni and Morris found that inertia magnifies the microstructural anisotropy and increases the grains’ contribution to the effective viscosity. To assess the significance of inter-grain interactions and inertia of fluid and grains, Haddadi and Morris computed different stress mechanisms, and Rahmani et al. examined momentum balance in the fluid and solid phases for different flow regimes. Nevertheless, there remains limited understanding toward the
influence of enhanced inertia related to grains heavier than the fluid. Zhou and Prosperetti\textsuperscript{25} compared the results of solid-to-fluid density ratios between 2.5 and 10 at $Re_p = 20$ and 40 and found that an increased density ratio results in stronger and more frequent collisions between grains, leading to notable modifications in the grain distribution, velocity profile, and bulk stress.

Moreover, studies on suspensions of non-spherical grains are relatively scarce, mainly due to the difficulty of dealing with geometrically complex boundaries. Among non-spherical grain suspensions, fiber suspensions are the most extensively studied due to their wide industrial applications and the availability of simulation methods, such as slender body dynamics.\textsuperscript{24,29} Apart from slender grains, much of the literature on non-spherical grains in dense suspensions has focused on interactions dominated by inter-grain contacts. For example, the gear-like\textsuperscript{35} and ellipsoidal\textsuperscript{35} grains have been simulated using the discrete element method (DEM) considering short-range repulsive contact forces. However, even though collisional interaction is rare in dilute regimes, Daghooghi and Borazjani\textsuperscript{27} have shown that there are still differences in rheology between suspensions of irregular-shaped and simple-shaped grains.

Considering the apparent gap in the literature as summarized above, the aim of this paper is to investigate the role of inertia and grain shape on the rheology of suspensions. Specifically, the contribution of fluid, grain–fluid hydrodynamics, and inter-grain collisional forces. However, even though collisional interaction is rare in dilute regimes, Daghooghi and Borazjani\textsuperscript{27} have shown that there are still differences in rheology between suspensions of irregular-shaped and simple-shaped grains.

The discretized momentum conservation equation is written as

$$
dv_i = - \sum_j m_j \frac{p_i + p_j}{p_i \cdot p_j} \nabla_i W + \sum_j m_j \frac{4\gamma_0}{(p_i + p_j)} \frac{|\mathbf{x}_i - \mathbf{x}_j|}{|\mathbf{x}_i|} \cdot \nabla_j W + \sum_j m_j \frac{|\mathbf{x}_i - \mathbf{x}_j|}{|\mathbf{x}_i|} \cdot \nabla_i W + g. \tag{3}
$$

The first term on the right-hand side of Eq. (3) is a symmetric balanced form of the pressure term\textsuperscript{35} where $p_i$, $m_i$, and $v_i$ denote the particle density, mass, and pressure, respectively. $\nabla_i W$ is the gradient of kernel function with respect to $\mathbf{x}_i$. The second and third terms represent the viscous stress\textsuperscript{35} and sub-particle-scale (SPS) stress,\textsuperscript{35} respectively, where $\gamma_0$ is the fluid kinematic viscosity and $\nabla_i W$ is the SPS stress tensor, which introduces the effect of turbulent motion at smaller scales than the kernel scale. $g$ is the gravitational acceleration.

To avoid solving the Poisson pressure equation, the equation of state is employed to find the pressure

$$
p_i = \frac{\rho_0 \gamma_0^2}{\xi} \left( \frac{p_i}{\rho_0} \right)^\xi - 1, \tag{4}
$$

where $\rho_0$ is a reference density at the initial state and $\xi = 2$ typically for incompressible fluids. $\xi_0$ is an artificial sound speed which should be set at least 10 times of the maximum fluid velocity to guarantee fluid density fluctuations below 1%.

The continuity equation is discretized as

$$
d\rho_i \over dt = \sum_j m_j (v_i - v_j) \cdot \nabla_i W + 2\delta c_0 \sum_j m_j (p_i - p_j) \frac{|\mathbf{x}_i - \mathbf{x}_j|}{|\mathbf{x}_i - \mathbf{x}_j|^2 + 0.01 h^2}, \tag{5}
$$

where the second term of the right-hand side is a diffusive term\textsuperscript{35} introduced to stabilize the density field during high-frequency oscillations. The parameter $\delta$ is set to 0.1 in this study.
In addition, the particle shifting technique is used to evenly distribute SPH particles in the whole domain, especially at the solid–fluid moving interfaces, and to prevent numerical cavity.

B. SPH-DEM coupling

Following the work of Koshizuka et al., the rigid DEM grain $I$ is also discretized by a series of SPH particles for SPH-DEM coupling, as shown in Fig. 1. The motion of DEM grains is governed by the Newton’s second law,

$$M_I \frac{dV_I}{dt} = \sum_{k \in I} m_k \frac{dV_k}{dt}$$

I

$$I_I \frac{d\Omega_I}{dt} = \sum_{k \in I} m_k (x_k - x_I) \times \frac{dV_k}{dt},$$

where grain $I$ possesses the mass $M_I$, velocity $V_I$, moment of inertia $I_I$, angular velocity $\Omega_I$, and center of gravity $X_I$. The right-hand side of Eq. (6) is the resultant force on grain $I$ summed from the unit forces applied to each discretizing particle (with mass $m_k$, position $x_k$, and velocity $v_k$), which mainly include (1) the body force (i.e., gravity), (2) the hydrodynamic force exerted by fluid particles, and (3) the contact force from other DEM grains. Since the rigid grains are discretized by ordinary SPH particles, the hydrodynamic force on a solid particle $k$ can be calculated following the same manner in SPH using Eq. (3). The calculation of contact force from other DEM grains is detailed in the following.

The normal contact force is given by a modified, non-linear, Hertzian model,

$$F_n = k_n \delta_n^{1.5} - \gamma_n^{0.25} \delta_n^n$$

where $k_n$ is the normal contact stiffness, $\delta_n$ is the interparticle overlap, $n$ is the unit normal vector at the contact, and $\gamma_n$ is the normal damping ratio. The first exponent 1.5 is derived for contacts between 3D spheres but also roughly applicable for 2D simulations. Hunt and Crossley suggested its range of $[1, 1.5]$ for the contact between two parallely aligned cylinders. The stiffness and damping ratio are given by Canelas et al.,

$$k_n = \frac{4}{3} E \sqrt{R},$$

where $E$ is the Young modulus, $\nu$ is Poisson’s ratio, $\mu$ is the friction coefficient, and $\epsilon$ is the coefficient of restitution. Table I lists the DEM parameters used in all the tests presented in this study.

Regarding the tangential contact force, the Coulomb law is modified with a sigmoidal function to render the force continuous with the tangential velocity,

$$F_t = F_t^{\text{prev}} + k_t \delta_t - \gamma_t \dot{\delta}_t,$$

where $F_t^{\text{prev}}$ is the previous tangential force, $k_t$ is the tangential contact stiffness, $\delta_t$ is the relative tangential displacement, $\gamma_t$ is the tangential damping ratio, and $\mu$ is the friction coefficient.

Adaptive time steps are calculated according to the Courant–Friedrichs–Lewy (CFL) condition as below

$$\Delta t = C \times \min \left( \frac{h}{|F_i|}, \frac{h}{c_0 + \max_i \sqrt{\frac{k_n}{M_i^2}}}, \frac{\pi}{50 \sqrt{k_n / M_i^2}} \right),$$

where the CFL coefficient is set to $C = 0.2$ in the study to guarantee numerical stability. The first term on the right-hand side is based on the force per unit mass ($F_i$) applied on the SPH particle $i$, the second term combines the CFL condition and the viscous time step control, and the third term is the constraint of DEM stability.

### Table I. DEM parameters in the coupled SPH-DEM simulations.

<table>
<thead>
<tr>
<th>Young’s modulus $E$ (Pa)</th>
<th>Poisson’s ratio $\nu$</th>
<th>Friction coefficient $\mu$</th>
<th>Coefficient of restitution $\epsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^8$</td>
<td>0.2</td>
<td>0.45</td>
<td>0.6</td>
</tr>
</tbody>
</table>

FIG. 1. Illustration of SPH discretization of fluid domain and solid grains.
coupling algorithm is illustrated in Fig. 2. The main calculation steps are parallelized and executed on GPU, which is a welcome feature available in DualSPHysics.

III. VALIDATION

To validate the fully resolved SPH-DEM model for fluid–grain mixture flows, five benchmark tests including water entry of a disk, sedimentation of an ellipse in a vertical channel, periodic flow around a sunflower-shaped object, pair-disk trajectories in a shear flow, and settlement of two vertically aligned disks have been conducted and compared with the available experimental and numerical results from the literature. All the simulations in the study are performed in 2D.

A. Water entry of a disk

The water entry problem of a disk is simulated with the SPH-DEM method. The problem was experimentally investigated by Greenhow and Lin⁴¹ and later modeled using the constrained interpolation profile (CIP) method by Zhu et al.⁴² The disk has a diameter \( D = 0.125 \) m and is dropped at a height of 0.5 m above the water surface, as shown in Fig. 3. The water depth is 0.3 m. The solid-to-fluid density ratio is either 0.5 or 1, corresponding to the half-buoyant or neutrally buoyant case, respectively. Sensitivity analysis on discretization is performed considering different initial SPH particle spacing \( d_p \) (i.e., \( d_p/D = 1/20, 1/25, \) and \( 1/40 \), respectively).

Figure 4 gives the evolution of water-entry depth in both half-buoyant and neutrally buoyant cases, comparing the present SPH-DEM results with those from the experimental⁴¹ and CIP⁴² studies. The SPH-DEM results converge to the CIP simulation and experimental results with the refinement of discretization. Specifically, when \( d_p/D \) is no greater than 1/25, the SPH-DEM and CIP methods have comparable performances and both correctly capture the evolution of water-entry depth in the two buoyant cases. Therefore, the initial SPH particle spacing is set to be \( d_p/D = 1/25 \) in the following tests. It is also observed that the disk de-acceleration is slower when its density is larger. At the entry depth of 0.3 m, the neutrally buoyant disk rebounds after it comes into contact with the container bottom.

B. Sedimentation of an ellipse in a vertical channel

A tilted ellipse falling under gravity in a closed vertical channel fully filled with fluid is considered. The problem configuration is
shown in Fig. 5. The domain width and height are \( L \) (0.004 m) and 17.5\( L \), respectively. The ellipse has an aspect ratio \( AR = 0.5 \) and its major diameter is \( L/4 \) (i.e., the blockage ratio is 4). Its center is initially 2.5\( L \) below the top surface with an inclination angle of 45°. The solid-to-fluid density ratio is 1.5. The initial SPH particle spacing is \( d_p = L/104 \).

Figure 6 plots the horizontal position and orientation of the ellipse vs the vertical position, respectively. Reasonable agreements are observed in comparison with the LBM results of Xia et al.\(^{43}\), IB-LBM results of Suzuki and Inamuro,\(^{44}\) and incompressible SPH (ISPH) results of Khorasanizade and Sousa.\(^{45}\)

C. Periodic flow around a sunflower-shaped object

Aiming to demonstrate the SPH-DEM capability in coping with complex geometries with sharp concave corners, the flow around a 13-petal sunflower-shaped object is analyzed. This test was described in Pan et al.,\(^{46}\) consisting of periodic flow through a plane channel with dimension 0.1 x 0.1 m\(^2\) and a sunflower-shaped body fixed at the center. Flow is driven by a body force of 1.5 \( \times 10^{-3} \) m/s\(^2\) imposed in the longitudinal x-direction. The initial SPH particle spacing is set to \( d_p = 0.0005 \) m, same as in Pan et al.\(^{46}\)

A steady flow solution is obtained for the specified conditions. The contour of longitudinal velocity is portrayed in Fig. 7, along with the result from Pan et al.\(^{46}\) A good agreement is found between the two studies from the comparison. More detailed assessment is performed in Fig. 8, where the longitudinal velocity profiles along the transverse y-direction are displayed at two distinct locations: across the center of the object (i.e., \( x = 0.05 \) m) and at the outlet boundary (i.e., \( x = 0.1 \) m). The present results agree well with both the SPH and finite element method (FEM) predictions reported by Pan et al.\(^{46}\)

D. Pair-disk trajectories in a shear flow

In this subsection, the pair-disk trajectories in a Newtonian fluid are studied. This case is relevant to suspension flows where hydrodynamic interactions are of primary importance. The problem is schematically shown in Fig. 9 with the same geometric parameters as in Choi et al.,\(^{47}\) i.e., the domain length \( L = 4 \) and width \( H = 1 \) (in the simulation, 1 length unit corresponds to a physical length of 0.12 m). Two equally sized \( (R = 0.1) \) smooth disks are freely suspended in a linear shear flow, and their initial positions are \( (L_x; L_y) \) and \( (L_x; -L_y) \) with \( L_x = 0.5 \) fixed in the study. The top and bottom walls move at opposite constant velocities to generate a laminar Newtonian flow with periodic boundary condition applied in the shear direction. The Reynolds number is measured to be about \( Re_p = 0.0288 \) [see Eq. (17)] so that the inertia effect is regarded as negligible. The original SPH particle spacing is \( d_p = L/600 \).

Trajectories for varying initial vertical positions of the two disks \( (\pm L_y) \) are depicted in Fig. 10, compared with the available FEM
It shows that the two disks repel each other and their trajectories are reversed like U-turns when their initial separations are small (e.g., \(L_y = 0.02\), 0.04, and 0.06). However, the two disks keep going in their sheared directions and pass each other when their initial separations become larger (e.g., \(L_y = 0.08\) and 0.10). The comparisons exhibit good match between the present SPH-DEM and existing FEM predictions, implying that the hydrodynamic forces are accurately computed when the particles get close. The minor difference between the two studies may be attributable to the small inertia effect (\(Re_p\) slightly larger than 0) and particle artificial roughness resulting from discretization in this study.

### E. Settlement of two vertically aligned disks

To further demonstrate the predictive capability of the proposed SPH-DEM for inter-grain collision problems, the settlement of two disks in a closed container filled with Newtonian fluid is investigated. The two disks have identical density and radius and are originally vertically aligned with some offset and released from rest. The model parameters are summarized as follows: the domain length 2 cm and height 6 cm, disk radius 0.125 cm and initial center positions (1 cm, 4.5 cm) and (1 cm, 5 cm), solid-to-fluid density ratio 1.5, fluid kinematic viscosity \(10^{-6}\) m²/s, and initial SPH particle spacing \(d_p = 0.00625\) cm.

The drafting–kissing–tumbling (DKT) phenomenon is clearly displayed in Fig. 11 at different time instants. First, the trailing disk catches up with the leading one due to reduced drag in the wake of the leading disk (\(t = 0.15\) s). Next, the two disks are close enough to be almost touching, corresponding to the kissing stage (\(t = 0.2\) s). Nevertheless, the contact is unstable and will be broken easily, leading to the tumbling of the two disks (\(t = 0.3\) s).
Figure 12 presents the evolution of vertical position and velocity of the two disks, comparing with the FDM results of Glowinski et al.\textsuperscript{17} and IBM results of Uhlmann.\textsuperscript{48} The present results are generally in good agreement with existing ones, except for some deviations in the tumbling separation stage as expected. The difference mainly arises from the distinct grain collision strategies adopted in these numerical methods. Glowinski et al.\textsuperscript{17} and Uhlmann\textsuperscript{48} simply considered a short-range repulsive force in the normal direction to prevent inter-grain penetration, whereas the contact model adopted in this study is more accurate in describing the collision behavior considering contact forces in both normal and tangential directions.

IV. SUSPENSION FLOW

In this section, suspensions of monodisperse solid disks of radius $R$ confined between two parallel no-slip walls are simulated to analyze their viscometric behavior under constant shear rate. Gravity is ignored in the simulation. The computational domain has a size $L$ in the flow direction ($x$) and a width $H$ in the gradient direction ($z$). The size relations are $L = 2H = 100R$. The $x$-directed shear flow is generated by moving the top wall with a speed of $U_w$ so that the equivalent shear rate is $\dot{\gamma} = U_w / H$. The periodic boundary condition is applied in the $x$ direction. The 2D solid fraction is denoted by $\phi$. In addition, two dimensionless numbers are used to describe the inertia effect of suspensions. The particle Reynolds number is defined as the ratio of the fluid inertial stress to the fluid viscous stress,

$$Re_p = \frac{4R^2\dot{\gamma} \rho_s}{\mu_f},$$

where $\rho_s$ and $\mu_f$ are the fluid density and dynamic viscosity, respectively. Another important parameter characterizing the suspension behavior is the Bagnold number, defined as the ratio of the grain inertial stress due to collision to the fluid viscous stress,\textsuperscript{49,50}

$$B_a = \frac{R^2 \rho_s}{1 - \phi} \mu_s = \frac{\phi}{1 - \phi} \frac{\rho_s}{\rho_f} Re_p,$$  \(18\)

where $\rho_s$ is the solid grain density. It is seen from Eq. (18) that the solid fraction, density ratio, and particle Reynolds number all contribute to the suspension flow properties. Hence, their effects will be examined separately in the following.

By varying the grain number (i.e., solid fraction), density ratio, and shear rate, different particle Reynolds and Bagnold numbers can be realized, resulting in different inertia effects of suspension flows. To further consider the influence of grain shape, suspensions of elliptic and sunflower-shaped grains are simulated for comparison, where two shape descriptors, i.e., aspect ratio and convexity, are used for quantitative analysis. These grains have the same area as the circular ones with an equivalent radius equal to $R$. The grain convexity (CV) is...
defined as its area divided by the area after filling all the concavities in its perimeter.\textsuperscript{51}

The model parameters of different test cases are summarized in Table II. Results are collected and analyzed after the mixture flow reaches a statistically steady state, as shown in Fig. 13. The shear stress $\tau$ is directly obtained from the shear force acting on the boundary walls, and the effective viscosity of the suspension is calculated from

$$\mu_s = \frac{\tau}{\dot{\gamma}}.$$  \hfill (19)

Sensitivity analysis on the effect of SPH particle discretization is conducted for a typical high-concentration ($\phi = 47\%$ and $Re_p = 0.15$) suspension of circular grains, considering $d_p/D = 1/15, 1/20, 1/25, 1/30, \text{ and } 1/35$, respectively. The evolution of relative viscosity $\mu_r$, defined as the ratio of effective viscosity of the suspension to that of the fluid, i.e., $\mu_r = \mu_s/\mu_f$, is shown in Fig. 14, which suggests apparent convergence of the results as $d_p$ decreases. In particular, when $d_p/D$ decreases from $1/30$ to $1/35$, the deviation of results is smaller than $5\%$. Therefore, $d_p$ is set to $D/30$ in the tests of this section, which strikes a good compromise between numerical efficiency and accuracy.

A. Relative viscosity

Figure 15 illustrates the relative viscosity flow curves for suspensions of circular grains with different ranges of solid concentration and density ratio. The shear-thickening phenomenon is observed in all cases as $\mu_r$ increases steadily with $\dot{\gamma}$, especially for large solid concentrations.
concentrations (e.g., $\phi \geq 36\%$) when the upsurge of viscosity with $\dot{\gamma}$ becomes noteworthy. The non-Newtonian behavior becomes more distinct with larger $\phi$ and density ratio. With $\rho_s/\rho_f$ increasing from 2.65 to 10, the viscosity flow curves for the two solid fraction cases $\phi = 25\%$ and $36\%$ shift upward. Zhou and Prosperetti reported similar observations for suspensions of noncolloidal particles albeit with larger Reynolds numbers in their study.

The dependence of $\rho_r$ on solid concentration $\phi$ for suspensions of both circular and non-circular grains with $\rho_s/\rho_f = 2.65$ is shown in Fig. 16. Results are presented together with the experimental data of Zarch et al. for soil–water mixture with $\rho_s/\rho_f = 2.62$ and $10^{-3} < Re_p < 10$, Mueller et al. for mixture of silicone oil and glass beads with $\rho_s/\rho_f = 2.74$ and $Re_p < 10^{-6}$, and numerical data of Gallier et al. with neutrally buoyant Stokes suspensions of spheres. The volume fraction in 3D suspensions is transformed to the area fraction by multiplying 3/2 according to previous studies for comparison between 2D and 3D results. It is evident from Fig. 16 that $\mu_r$ increases at a greater rate with larger $Re_p$ which partly explains the more rapid increasing $\mu_r - \phi$ curve in Zarch et al. compared to the results of Gallier et al. and Mueller et al. The curve of $Re_p = 0.3$ in the present study fits well with the data of soil–water mixture in Zarch et al. In addition to the role of inertia, the grain shape also has a significant impact on the non-Newtonian flow property. At the same $Re_p$ and $\rho_s/\rho_f$, a prominent increase in $\rho_r$ is found with decreasing AR and CV. The effects of inertia and grain shape will be further explored in Secs. IV B–IV E.

B. Stress contributions

The different roles of inertia and grain shape on suspension viscosity can be better understood by studying their contributions to the overall shear stress. We implemented the procedure developed by Batchelor to calculate the bulk stress generated by a flowing suspension in terms of area averages. The relative viscosity can be written as:

$$\mu_r = \frac{\tau}{\dot{\gamma}}$$
where $\Sigma_{xz}^*$ represents the grain-induced stress defined as follows:

$$\Sigma_{xz}^* = \frac{1}{\mu_T^*} \left( S_{xz} + \hat{S}_{xz}^* \right) - (1 - \phi)\Re_p \left( \vec{u}_{xz}^* \vec{u}_{xz}^* \right),$$

(21)

where $\mu_T^*$ denotes the ensemble averaged quantity. The first term on the right-hand side denotes the hydrodynamic and collisional stresslets defined by

$$s_{xz} = \frac{1}{2\Re} \sum \left( r_{xz}^f + r_{xz}^c \right),$$

(22)

where $r_{xz}^f$ and $r_{xz}^c$ (i.e., $x = x$ or $z$) are the hydrodynamic force and inter-grain collisional force exerted on the grain, respectively; $\Re$ is the branch vector connecting the grain centroid and the point of force application. The summation is carried out over all the grains. The last two terms represent the Reynolds stress from fluctuations of grains and fluid particles. The acceleration stress is ignored in the study due to its insignificant contribution. The velocity fluctuations of grain and fluid ($\vec{u}_{xz}^*$) are calculated as $\vec{u}_{xz}^* = \vec{u}_{xz} - \vec{u}_{xz}^f$ and $\vec{u}_{xz}^f = \vec{u}_{xz} - \vec{u}_{xz}^c$, where $\vec{u}_{xz}$ is the undisturbed velocity for a uniformly sheared fluid. The Reynolds stress cannot be ignored when the bulk Reynolds number is out of the range of laminar flows.

The relative viscosity obtained from both the shear stress on the walls [i.e., Eq. (19)] and the bulk stress calculated using Eq. (20) for different cases is displayed in Fig. 17. The two measures show an over-all reasonable agreement although there is a deviation of about 7% for the AR = 0.66 case which owes to the increased boundary effect as to be shown in Fig. 23(a), consistent with the findings in Kulkarni and Morris.

The contributions of each term (i.e., fluid viscous stress, grain hydrodynamic stress $s_{xz}$, collision stress $\hat{S}_{xz}^*$, and Reynolds stress) to the overall viscosity are evaluated for various $Re_p$ and $\phi$ in Fig. 18. Irrespective of $Re_p$, the contributions from both grain hydrodynamics and collision increase, resulting in an increase of total relative viscosity. The grain-related stress $(s_{xz} + \hat{S}_{xz}^*)$ is dominant to the total stress when $\phi \geq 36\%$. More specifically, for $14\% \leq \phi \leq 36\%$, the contribution of particle-fluid interaction ($s_{xz}$) plays a leading role in the enhancement of overall viscosity. However, the collision $(\hat{S}_{xz}^*)$ contribution to viscosity significantly rises when $\phi$ increases from 36% to 47% and eventually occupies 39.5% of the overall viscosity in the case $Re_p = 0.45$. The inter-grain collision, therefore, accounts for the exponential growth of $\mu$, presented in Fig. 16.
By comparing the results of different $Re_p$ in Fig. 18, it is found that increasing $Re_p$ leads to the rising of both hydrodynamic and collision stresses. The inter-grain collision contribution increases dramatically with the growth of $Re_p$, especially for $\phi \geq 36\%$, which may explain the more significant shear-thickening phenomenon for $\phi \geq 36\%$ in Fig. 15.

Figure 19 indicates that the grain-related contribution ($\Sigma_{xz}$) to viscosity is affected by grain density for both $\phi = 25\%$ and 36\% cases. As grain density becomes larger, both collision and grain hydrodynamics show a gradual rise while Reynolds stress caused by disturbance of grains enhances greatly, especially at large $Re_p$. It well explains the observation in Fig. 15. In spite of the surge of velocity fluctuations caused by grain inertia, the contribution of Reynolds stress to the total stress is generally below 15% and the flow is still in the inertial shear-thickening regime, far from the turbulent-like regime.

The rheology of suspensions with elliptic and sunflower-shaped grains is investigated to explore the influence of grain shape. Figure 20(a) shows that as AR decreasing, the grain-related stress ($\Sigma_{xz} + \sigma_{xz}^G$) grows which results in the steady increase of total relative viscosity, whereas AR has less significant effect on Reynolds stress. Moreover, the effect of AR on inter-grain collision intensifies for larger $Re_p$. Conversely, the contribution from grain hydrodynamics increases when AR decreases from 1 to 0.66 and remains roughly constant with further decreasing of AR. The role of CV to the relative viscosity of suspension is displayed in Fig. 20(b). A growth of particle-related contribution is found as CV decreases. Such increases are more notable when CV drops from 1 to 0.91 and from 0.84 to 0.74, compared with...
that when CV varies in the range between 0.91 and 0.84, which exhibits a similar trend as average grain rotation to be shown in Fig. 28(b). More specifically, the marked growth from CV $\equiv 1$ to 0.91 is mainly due to the increase of fluid–grain interactions ($s_{xz}$) for both $Re_p$. As CV decreases from 0.84 to 0.74, the surging velocity fluctuations resulting from grain concavity play a significant role in the increase of bulk viscosity.

C. Profiles of solid concentration and velocity

The solid concentration profile is first presented to characterize the grain layering and the near-wall effects on suspension flows, as it is possible cause to shear-thickening of suspensions. This is achieved by dividing the computational domain into 250 equally sized layers parallel to the walls and calculating the time-averaged solid area fraction in each layer during the steady state.

A local concentration peak near the stationary wall ($z/H = 0$) is clearly visible with $\phi = 47\%$ for the case $Re_p = 0.45$ and $\rho_s/\rho_f = 2.65$ shown in Fig. 21, though not as pronounced as in 3D systems reported elsewhere.\(^{11}\) The formation of stable solid layers near the wall may be resulted from the strong grain–wall interaction. The local concentrations grow to the bulk concentration values faster and peaks closer to the wall as $\phi$ increases, in agreement with the results of Kromkamp et al.,\(^{11}\) Picano et al.,\(^{58}\) and Yeo and Maxey.\(^{59}\) Figure 22 presents the flow profiles for $\phi = 36\%$ with different $Re_p$ and $\rho_s/\rho_f$, indicating that the local solid fraction tends to rise slightly faster and higher with increasing $Re_p$ and grain density. Nevertheless, $Re_p$ and grain density play an insignificant role in the distribution of local solid fraction in the bulk region away from the boundary walls, which is consistent with the finding in Zhou and Prosperetti.\(^{22}\)

![FIG. 20. Contributions of Reynolds stress, inter-grain collision, grain hydrodynamics, and fluid viscosity to overall viscosity with different grain shapes: (a) aspect ratio and (b) convexity.](image)

![FIG. 21. Time-averaged solid area fraction across the domain width with varying bulk concentrations for suspensions of circular grains.](image)

![FIG. 22. Time-averaged solid area fraction across the domain width with varying $Re_p$ and $\rho_s/\rho_f$ for suspensions of circular grains.](image)
In addition, to show the influence of grain shapes, the flow profiles for $\phi = 36\%$, $Re_p = 0.30$, and $p_s/p_f = 2.65$ with varying AR and CV are displayed in Fig. 23. The local concentration near the stationary wall increases as both AR and CV deviate from unity. However, the three cases with CV in the range between 0.91 and 0.74 show similar near-wall peak concentration values.

Additionally, the velocity profiles of fluid (nearly identical for solid grains) for different solid concentration, inertia, and shape of grains are shown in Fig. 24 to further explore the influence of wall effect. Near the two walls ($0 < z/H < 0.04$ and $0.96 < z/H < 1$), the slopes of the curves are steeper than the 1:1 reference line. The enhancement of velocity gradient is more pronounced in higher solid concentration and smaller aspect ratio and convexity cases, where strong layering of grains near the walls is also observed. It seems that the presence of grains near the wall may create a region of increasing velocity gradient, known as the slip layer. The smaller velocity gradient in the bulk of the system (i.e., away from the walls) explains the lower bulk stress than the wall stress presented in Fig. 17.

D. Pair microstructure

The pair microstructure is characterized by the pair distribution function $g(r, \theta)$ defined as the probability of finding a grain at the distance $r$ and polar angle $\theta$ to a given grain. Particularly, the probability of the nearest neighbors, i.e., $2R < r < 2.1R$, is examined in the study.

As previously shown in Fig. 10, the pair-particle trajectories are fore-aft symmetric in the dilute pure hydrodynamic limit ($Re_p \approx 0$) owing to the reversibility of Stokes equations. However, the symmetry can be broken by the Brownian motion, inter-grain contacts, and finite inertia. In this study, the effects of the latter two factors are analyzed as presented in Figs. 25 and 26 with varying $Re_p$, $\phi$, $p_s$, and CV. Considering the radial symmetry, only results in the range $0 < \theta < 180^\circ$ are shown.

As shown in Fig. 24, the pair distribution functions exhibit a clear asymmetric pattern with elevated probability density in the compressional quadrant ($\theta > 90^\circ$) and a marked depletion zone around the extension axis. When $\phi$ increases, there are accumulating probabilities.

![FIG. 23. Time-averaged solid area fraction across the domain width with varying (a) aspect ratio and (b) convexity.](image)

![FIG. 24. Time-averaged velocity profiles across the domain width with varying (a) solid concentration and $Re_p$ and (b) grain shape.](image)
for a given grain to encounter another one in the compression zone and along the shear direction \((\theta \approx 0^\circ)\). The probabilities in the compression zone also increase with \(Re_p\), especially at low \(\phi\). The effect of \(Re_p\) however, diminishes with \(\phi\) as seen from Fig. 25(d) that the pair distributions are close when \(Re_p\) increases from 0.15 to 0.45 at \(\phi = 47\%\). To further explore the role of particle inertia, pair distribution functions for suspensions of different density ratios \((\rho_s/\rho_f = 2.65\) and 10\) are also presented in Figs. 25(a)–25(c). Similar to the influence of \(Re_p\), the increase of grain density magnifies the anisotropy in the pair microstructure and fore-aft asymmetry.

The influence of grain convexity is further examined. As seen from Fig. 26 that the chance to find a neighbor at around \(2R\) for a given grain in the compression zone is reduced with decreasing \(CV\), which is especially evident when \(CV\) drops from 0.91 to 0.84. It is probably because of the additional excluded areas near contact due to grain concavities.

**E. Grain rotation**

Grain rotation plays an equally important role in the interactions among grains and between grains and fluid. The grain rotation is measured by \(\Omega^*\) defined as the mean grain angular velocity \(\Omega\) normalized by the bulk shear rate of the mixture, i.e., \(\Omega^* = \Omega/\gamma\).

For the results of circular grain suspensions presented in Fig. 27, \(\Omega^*\) decreases with increasing \(\phi\) for all Reynolds numbers, in agreement with previous studies.\(^8\) It can be understood that higher volume fraction leads to more significant constraints from neighbors on grain rotation. The comparisons between different grain density \(\rho_s\) for \(\phi = 25\%\) and 36\% show reduced grain rotation at higher \(\rho_s\). Similarly, grain angular velocity declines as Reynolds number rises in accordance with that reported by Mikulencak and Morris\(^9\) using data collected from the literature. It may be attributed to the enhanced inter-grain contacts at large \(Re_p\) that suppresses the shear-induced grain rotation.
The reduction in grain rotation at higher $Re_p$ has resulted in the rise of shear stress or viscosity of the suspensions because of the steeper velocity gradients of interstitial fluid.

Figure 28 shows the normalized average grain rotation in suspensions with non-circular grains at $\phi = 36\%$ and $\rho_s/\rho_f = 2.65$ and 10. Regardless of the particle Reynolds number, grain rotation decreases monotonically with both decreasing AR and CV although at different declining rates. The drop is faster with respect to decreasing AR and the trend is accelerating. Contrarily, a mild descent of grain rotation is observed with decreasing CV, especially when CV becomes smaller than 0.91, which is similar to the increasing trend of relative viscosity in Fig. 20(b). Moreover, the rate of descent is repressed by inertia which results in flatter curves when $Re_p$ increases from 0.3 to 4.5.

Based on the above analyses, it can be concluded that grain shape has a significant impact on the viscosity of suspensions due to the interplay among inter-grain collisions, fluid–grain interactions, and the non-uniform flow profiles. Grains with lower AR or CV tend to have a larger surface area and can, thus, intensify inter-grain and fluid–grain interactions. Specifically, concave grains increase the grain hydrodynamic stresslet by augmenting fluid–grain interactions. Contrarily, the grain hydrodynamics first increases with decreasing AR before declining, possibly because grains with lower AR are more likely to align with the flow direction. When the Reynolds stress becomes non-negligible, concave particles play a more significant role in perturbing the flow field while AR has less impact. Moreover, both AR and CV can suppress grain rotation, leading to higher shear stresses.

V. CONCLUSIONS

The rheology of 2D fluid–grain mixtures in a Couette flow has been studied using a fully resolved SPH-DEM method, with an emphasis on the roles of inertia and grain shape. The model has been rigorously validated through several benchmark problems, including water entry of a disk, sedimentation of an ellipse, periodic flow around a sunflower-shaped object, pair-disk trajectories in a shear flow, and the DKT phenomenon of two settling disks. The test results have adequately verified the accuracy of the present SPH-DEM method in simulating grain–fluid hydrodynamic interaction and inter-grain collision, as well as in dealing with complex grain shapes. The main findings from the study are summarized below.

(1) In the macroscale, the suspension effective viscosity intensifies with increasing particle Reynolds number $Re_p$, solid concentration $\phi$, and solid-to-fluid density ratio $\rho_s/\rho_f$, leading to more pronounced shear-thickening behavior. Additionally, suspensions of grains with lower AR and CV present greater effective viscosity.

(2) The transitional behavior of suspensions is analyzed by separating the contributions to the bulk shear stress. It is found that the increase of effective viscosity is mainly attributable to the enhancement of fluid–grain hydrodynamic interaction, inter-grain collision, and Reynolds stress, whereas the contribution from fluid viscous stress remains largely unaltered with increasing $Re_p$, $\phi$, and $\rho_s/\rho_f$. Additionally, the contribution of Reynolds stress magnifies when the inertia increases.
The elongation and concavity of suspended grains will also increase both the particle-fluid hydrodynamic and inter-grain collision contributions to the overall effective viscosity. The grain concavity will intensify the Reynolds stress when the inertial effect becomes nonnegligible. (3) Grain clustering is found near the walls in suspension flows. Inertia and grain elongation and concavity will increase the solid concentration near walls. As for near contact pair structures, the fore-aft symmetry breaks in the sheared suspension flow. Such asymmetry becomes more evident as Re, φ, or ρ increases or grain convexity decreases.

(4) Average particle angular velocities show dependence on Re, φ, ρ, AR, and CV. Grain rotations are suppressed by increasing inertia and non-circular grain shapes. The microstructural anisotropy and grain kinematics characteristics play a crucial role in the shear-thickening behavior observed in noncolloidal suspension flows.

Although microscopic analyses are presented in the study, there is still a need for quantitative correlations between the macroscopic viscosity and microscopic quantities such as pair distribution, grain rotation, and grain shape. It is possible to develop such correlations by extending existing semi-empirical formulas (e.g., Eilers formula), which will be explored in future studies.

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AUTHOR DECLARATIONS
Conflict of Interest
The authors have no conflicts to disclose.

Author Contributions
Yueting Li: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Investigation (equal); Software (equal); Validation (equal); Visualization (equal); Writing – original draft (equal). Ning Guo: Conceptualization (equal); Funding acquisition (equal); Methodology (equal); Project administration (equal); Resources (equal); Supervision (equal); Writing – review & editing (equal). Zhongxuan Yang: Conceptualization (equal); Funding acquisition (equal); Resources (equal); Writing – review & editing (equal). Jidong Zhao: Validation (equal); Writing – review & editing (equal).

DATA AVAILABILITY
The data that support the findings of this study are available within the article.

REFERENCES


