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1	A numerical study of the settling of non-spherical particles in quiescent water
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16 ABSTRACT

17 The settling of non-spherical particles is poorly understood, with previous studies 18 having focused mainly on spherical particles. Here, a series of particle-resolved direct 19 numerical simulations are conducted using FLOW-3D (commercial computational fluid 20 dynamics software) for spheres and five regular, non-spherical shapes of sediment 21 particles, i.e., prolate spheroid, oblate spheroid, cylinder, disk, and cube. The Galileo number varies from 0.248 to 360 and the particle Reynolds number Re_p ranges from 22 0.00277 to 562. The results show that a non-spherical particle may experience larger drag 23 and consequently attain a lower terminal velocity than an equivalent sphere. If Re_p is 24 25 sufficiently small, the terminal velocity is less affected by particle shape as characterized by the particle aspect ratio. For relatively large Re_p , the shape effect (represented by the 26 Corey shape factor) becomes more significant. Empirical correlations are derived for the 27 28 dimensionless characteristic time t_{95*} and displacement s_{95*} of particle settling, which show that t_{95*} remains constant in the Stokes regime ($Re_p < 1$) and decreases with 29 increasing Re_p in the intermediate regime $(1 \le Re_p < 10^3)$, whereas s_{95*} increases 30 progressively with increasing Re_p over the simulated range. It is also found that in the 31 32 Stokes regime, particle orientation remains essentially unchanged during settling, and so 33 the terminal velocity is governed by the initial orientation. In the intermediate regime, a 34 particle provisionally settling at an unstable orientation self-readjusts to a stable 35 equilibrium state, such that the effect of initial orientation on the terminal velocity is negligible. Moreover, an unstable initial orientation can enhance the vertical displacement 36 37 and may promote vortex shedding.

39 HIGHLIGHTS

40	•	Settling of non-spherical particles is investigated using commercial computational
41		fluid dynamics software.
42	•	At low particle Reynolds numbers, an increase in particle aspect ratio may
43		correspond to a reduction in terminal velocity.
44	•	The characteristic time remains constant throughout the Stokes regime and decreases
45		with increasing particle Reynolds number in the intermediate regime.
46	•	An unstable initial orientation may promote vortex shedding from particles settling
47		in the intermediate regime.
48		

49 I. INTRODUCTION

50 The settling of particles in fluids is key to many natural and industrial processes, such as sediment dynamics in alluvial rivers,^{1,2} transportation of marine microplastics,^{3,4} 51 proppant settling in hydraulic fractures,^{5,6} and chemical and powder processing.⁷ 52 53 Although particulate flows are generally turbulent and involve large amounts of particles, 54 an improved understanding of the settling of a single particle in quiescent fluid is a 55 prerequisite for modelling complex particle-laden turbulent flows. However, most 56 existing models of particulate flows assume the grains to be spheres when in fact the most commonly encountered particles in practical applications are non-spherical.^{8,9} Such 57 58 simplification inevitably ignores the key roles played by particle shape and orientation in 59 the settling process. Studies are urgently needed to gain better insight into the settling of 60 non-spherical particles in quiescent water.

When a heavy particle falls through a static fluid, the particle accelerates due to gravity and increasing fluid drag is exerted on its surface. As the submerged weight of the particle is balanced by fluid drag, its acceleration terminates, enabling the particle to fall at a nearly constant velocity, called the terminal velocity. The drag force is one of the fundamental forces that affect the settling process, which can be defined as

66
$$F_d = \frac{1}{2} C_d \rho_f W^2 \frac{\pi}{4} d_n^2, \qquad (1)$$

67 where C_d is the drag coefficient; ρ_f is the fluid density; W is the settling velocity; 68 and d_n is the diameter of a sphere of equivalent volume to that of the particle. Accurate 69 estimates of settling velocity and drag coefficient are of particular importance because 70 other parameters can be readily inferred. Notably, the terminal velocity of a particle, 71 denoted W_t , can be simply derived by equating the drag force to the submerged weight

of the particle. The drag coefficient C_d in Eq. (1) is however very challenging to 72 73 determine because it depends on many parameters including the particle Reynolds number and particle shape.¹⁰ Herein, the particle Reynolds number is defined as 74 $Re_p = Wd_n / v$, with v being the kinematic viscosity. Except at sufficiently small Re_p , 75 where an analytical solution exists for spheres based on Stokes' law, in which C_d is 76 inversely proportional to Re_p , no general solution can be found for determining the drag 77 78 coefficient of particles of any shape. Based on a large number of theoretical and 79 experimental investigations of settling behavior, numerous empirical models have been developed to predict the drag coefficient and settling velocity of spherical particles¹¹⁻¹³ 80 and non-spherical particles.¹⁴⁻¹⁸ To account for the shape effect of non-spherical particles, 81 82 various approaches have been proposed to define particle shape. Of these, the Corey shape factor¹⁹ (CSF) is the most commonly used shape descriptor,^{14,20,21} and is defined as 83 $\text{CSF} = d_s / \sqrt{d_m d_l}$, where d_s , d_m , and d_l are respectively the shortest, intermediate, 84 85 and longest form dimensions of the particle. Sphericity ϕ is another widely used shape descriptor,^{15,22,23} and is given by the ratio of the surface area of the volume-equivalent 86 87 sphere to that of the actual particle. Circularity X is the ratio of the perimeter of the 88 maximum projection area of the particle to the perimeter of a circle that has area equal to 89 the maximum projection area. This descriptor is able to reflect the irregularity of particle 90 contours and is thus very suitable for particles with sharp corners and large obtuse angles.²⁴ In addition, for highly irregular particles, the parameter ξ , which is the ratio 91 ϕ/X , is another effective shape descriptor.^{17,25,26} However, these aforementioned 92 93 empirical models cannot provide sufficient effective information to quantify the whole 94 process of particle settling. Consequently, the time and space scales that are required for 95 a particle to reach its terminal settling state have not yet been resolved.

96 Particle orientation also has a vital effect on settling non-spherical particles. In 97 general, a non-spherical particle could fall at any orientation without rotation at sufficiently small Re_p ,^{27,28} but will assume a stable orientation and tend to fall with the 98 99 maximum projection area normal to the direction of settling motion at relatively large Re_n .^{8,29} Besides, particle orientation can appreciably modify the drag coefficient.^{16,18} 100 101 Over the past decade, particle-resolved direct numerical simulation (PR-DNS) has been carried out to establish correlations between C_d and particle orientation.³⁰⁻³³ However, 102 103 such correlations are based on the assumption of a stationary obstacle exposed to a 104 moving fluid, therefore neglecting the effects of secondary motions and wake structures.³⁴ 105 Moreover, most existing numerical studies considering the influence of particle orientation on free settling have been confined to two-dimensional modeling.³⁵⁻³⁷ Overall, 106 107 there is a need for a three-dimensional model that can properly address the effect of 108 particle orientation on the settling process of non-spherical particles.

109 The present work sets out to unravel the effects of particle shape and initial 110 orientation on the settling of non-spherical sediment particles in quiescent water. Using 111 the commercial computational fluid dynamics (CFD) software FLOW-3D (version 11.2), 112 a series of PR-DNS simulations are performed for a range of particle sizes, shapes, and 113 distinct initial orientations. Based on the computational results, key parameters that characterize the settling process, including terminal velocity W_t and drag coefficient 114 C_d , are analyzed to reveal the influence of particle shape on settling. Furthermore, the 115 116 time and space scales required to reach terminal settling are also investigated. In addition, 117 the settling processes of non-spherical particles in the Stokes and intermediate regimes 118 are presented, thereby probing into the effect of initial particle orientation.

119 II. METHOD

120 A. Computational fluid dynamics (CFD) model

The commercial CFD software FLOW-3D, developed by Flow Science, is used to conduct PR-DNS simulations of particle settling in otherwise quiescent fluid. FLOW-3D utilizes a fractional area/volume obstacle representation (FAVOR) technique³⁸ and provides a general moving object model that can simulate rigid body motion that is dynamically coupled with fluid flow. The FAVOR method defines complicated geometric shapes through fractional areas and volumes within rectangular elements and has proven to be one of the most efficient methods to treat immersed solid bodies.^{39,40}

Assuming the fluid to be incompressible, the continuity and momentum equationsbased on the FAVOR method are given as

130
$$\frac{\partial U_i}{\partial x_i} = -\frac{\partial V_f}{\partial t},$$
 (2)

131
$$\frac{\partial u_i}{\partial t} + \frac{U_j}{V_f} \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_f} \frac{\partial p}{\partial x_i} + g_i + f_i, \qquad (3)$$

where subscripts *i* and j=1,2,3 denote *x*, *y*, and *z* directions; x_i are Cartesian coordinates; *t* is time; $U_i = u_i A_{\underline{i}} = (uA_x, vA_y, wA_z)$ in which u_i is the *i*-th velocity component and A_i is the corresponding area fraction; V_f is volume fraction; *p* is pressure; g_i is the *i*-th body acceleration component; and f_i is the *i*-th viscous acceleration component. The viscous acceleration components in Eq. (3) are calculated as

138
$$f_i = \frac{1}{\rho_f V_f} \left(wsx_i - \frac{\partial T_{ij}}{\partial x_j} \right), \tag{4}$$

139 where wsx_i are wall shear stress components; and $T_{ij} = A_{\underline{j}}\tau_{ij} = -2A_{\underline{j}}\mu(s_{ij} - s_{kk}\delta_{ij}/3)$, in 140 which μ is dynamic viscosity, $s_{ij} = (\partial u_i / \partial x_j + \partial u_j / \partial x_i)/2$ is the strain rate tensor, 141 and δ_{ij} is the Kronecker delta function. Compared to the continuity equation applied in 142 stationary obstacle problems, $-\partial V_f / \partial t$ on the right-hand side of Eq. (2) is equivalent to 143 an additional volume source term and exists solely in mesh cells around the boundary of 144 the moving object. The term is evaluated as

145
$$-\frac{\partial V_f}{\partial t} = \frac{S_{\rm obj}}{V_{\rm cell}} V_{\rm obji} n_i, \qquad (5)$$

146 where V_{cell} is the volume of a mesh cell; S_{obj} , n_i , and V_{obji} are respectively the 147 surface area, unit normal vector, and velocity of the moving object in the mesh cell. 148 According to kinematics, the general motion of a rigid body can be divided into

translational motion and rotational motion components. Newton's second law describesthe translational motion of a rigid body as

151
$$m_p \frac{d\mathbf{V}_G}{dt} = \mathbf{F},$$
 (6)

where \mathbf{V}_{G} is the mass center velocity of the rigid body; **F** is the total force on the body; and m_{p} is rigid body mass. Euler's equation describes rigid body rotation in a frame of reference fixed at the centroid of the rotating body as

155
$$\mathbf{I}\frac{d\boldsymbol{\omega}}{dt} + \boldsymbol{\omega} \times (\mathbf{I}\boldsymbol{\omega}) = \mathbf{T}_G, \tag{7}$$

where $\boldsymbol{\omega}$ is the angular velocity of the rigid body; I is the diagonal inertia matrix relative to the principal axes of the rigid body; and \mathbf{T}_{G} is the total torque about the mass center. The present paper considers the free settling of a single particle, so the total force and total torque include only hydrodynamic and gravitational forces and torques. 160 The CFD model solves the governing equations of fluid motion [Eqs. (2) and (3)] 161 using a finite volume/finite difference method.⁴¹ Pressures and velocities are coupled 162 implicitly and solved by using a generalized minimal residual method, which is the 163 default solver of FLOW-3D. The momentum advection algorithm adopts a first-order 164 upwind scheme. For coupled rigid body motion [Eqs. (6) and (7)], both the explicit and 165 implicit general moving objects methods work well since heavy object problems are 166 considered in the present paper.

167

168 B. Study cases

169 A series of numerical cases are used to investigate the influences of particle shape 170 and initial orientation on the settling of non-spherical particles. Table I summarizes the simulation parameters. In all cases, the fluid is specified as water at 20 °C ($\rho_f = 1000$ 171 kg/m³, $v = 1 \times 10^{-6}$ m²/s), and the particles are assumed to be composed of siliciclastic 172 173 sediment of homogeneous density 2650 kg/m³. Eight spherical equivalent diameters are considered, i.e., $d_n = 0.015625$, 0.03125, 0.0625, 0.125, 0.25, 0.5, 1, and 2 mm. 174 Consequently, the value of the Galileo number varies from 0.248 to 360. The Galileo 175 176 number Ga is the ratio between gravitational and viscous forces, and is defined as

177
$$Ga = \frac{\sqrt{\left|\rho_{p} / \rho_{f} - 1\right| gd_{n}^{3}}}{v}, \qquad (8)$$

178 where ρ_p is particle density; and g is gravitational acceleration. As indicated in Table 179 II, six particle shapes are considered, including spheres and five regular non-spherical 180 shapes, i.e., prolate spheroid, oblate spheroid, cylinder, disk, and cube, with the first four 181 shapes being axisymmetric. Although particles in natural and industrial processes are 182 generally irregular, it is justified to choose regular non-spherical particles as the object of 183 the present study because most accurate models for predicting the behavior of non-184 spherical particles in fluids have been based on studies on regular particles, for which the 185 characterization of the particle shape is not complex.¹⁸

186 Among the parameters listed in Table I, β is defined as the angle between the plane 187 in which the maximum projection area of a particle lies and the horizontal plane 188 perpendicular to the direction of settling motion (and thus provides a reasonable description of the particle orientation). β_0 denotes the initial orientation of a particle 189 190 upon release. As previously noted, a particle settling at sufficiently small Re_p exhibits 191 no preferred orientation. If Re_p is relatively large, a particle tends to fall with its 192 maximum projection area normal to the direction of settling motion, i.e., at a state of 193 $\beta = 0^{\circ}$. Therefore, the typical initial state of $\beta_0 = 0^{\circ}$ is chosen to exclude any influence 194 of orientation variation; the combination of different particle sizes and shapes leads to 36 cases. A further 32 cases that consider two distinct initial orientations ($\beta_0 = 45^\circ$ and 90°) 195 196 are simulated for axisymmetric particles with four selected spherical equivalent diameters $(d_n = 0.015625, 0.0625, 0.25, and 1 mm)$. Overall, a total of 68 numerical cases are 197 198 considered, and the particle Reynolds number Re_p ranges from 0.00277 to 562, covering both the Stokes regime ($Re_p < 1$) and the intermediate regime ($1 \le Re_p < 10^3$). 199

In this paper, the Corey shape factor CSF is used to describe particle shape, noting that CSF suffices for regular particles.⁴² The projection area protocol, which is associated with the lowest operator-dependent errors compared to other methods,⁴³ is applied to determine the form dimensions of a given particle (see Table II). Particle settling is simulated in a domain of dimensions $8d_n \times 8d_n$ in the *x* and *y* directions. The size of the domain in the *z*-direction is carefully determined to ensure the whole-process modeling 206 of particle settling can be achieved without exceptional computational cost. A resolution of 12 grids per d_n is used, which can successfully resolve the geometry of both spherical 207 208 and non-spherical particles considered in the present study. Periodic boundary conditions 209 are imposed in the horizontal directions to mimic an unbounded domain without wall 210 effect, and a free surface and a stationary wall are implemented at the upper and bottom 211 boundaries. More information on validation of the CFD model is given in the Appendix. 212 In addition, a dual-Euler whole-attitude solver is used to reproduce the variation in 213 orientation of particles, based on the time series of particle angular velocities output from 214 the CFD model. A brief description of the method is given in the Supplementary Material. 215

217	TABLE I. Summary of simulation parameters.					
	$\rho_f (\text{kg/m}^3)$	$\nu (m^2/s)$	$\rho_p \left(\text{kg/m}^3 \right)$	$d_n \pmod{mm}$	eta_0 (°)	
	1000	1×10 ⁻⁶	2650	0.015625-2	0, 45 and 90	
218						

TABLE II. Summary of six particle shapes considered in this work. Semi-axes lengths of the ellipsoid are a, b, and c; the diameter and height of the cylinder and disk are dand h (d < h for the cylinder, d > h for the disk), respectively; and the edge length of the cube is a.

Shape	d_{l}	d_{m}	d_s	CSF
Sphere	d_n	d_n	d_n	1.00
Ellipsoid 1 (prolate spheroid, $a = 4b = 4c$)	2 <i>a</i>	2 <i>b</i>	2 <i>c</i>	0.50
Ellipsoid 2 (oblate spheroid, $a = b = 2c$)	2 <i>a</i>	2 <i>b</i>	2 <i>c</i>	0.50
Cylinder $(h = 2d)$	$\sqrt{h^2+d^2}$	d	d	0.67
Disk $(h=1/4d)$	$\sqrt{h^2+d^2}$	d	h	0.25
Cube	$\sqrt{3}a$	$\sqrt{2}a$	а	0.64

225 III. RESULTS AND DISCUSSION

226 A. Particle settling with maximum projection area normal to fall direction

227 1. Terminal settling state

The terminal settling state and terminal velocity of a particle are simultaneously attained when the submerged weight of the particle is balanced by fluid drag. Terminal velocity is a fundamental hydrodynamic parameter that both directly and indirectly governs sedimentary processes.²⁹ Here, the terminal velocity W_t and spherical equivalent diameter d_n are normalized following Dietrich¹⁴, such that:

233
$$W_{t*} = \frac{\rho_f W_t^3}{\left(\rho_s - \rho_f\right) g \nu},\tag{9}$$

234
$$d_* = \frac{(\rho_s - \rho_f)gd_n^3}{\rho_f v^2},$$
 (10)

where W_{t*} is the dimensionless terminal velocity; and d_{*} is the dimensionless 235 spherical equivalent diameter. Figure 1 illustrates the variation in W_{t*} with d_{*} obtained 236 for different shapes when $\beta_0 = 0^\circ$. It appears that a non-spherical particle attains a lower 237 238 terminal velocity than its spherical counterpart, with the difference in terminal velocity 239 becoming increasingly evident as the particle size increases. This trend is further 240 confirmed in Figure 2 which shows the variation in δ with particle Reynolds number Re_p where δ is defined as the relative deviation of the terminal velocity of a non-241 spherical particle from that of its spherical counterpart with the same d_n as follows: 242

243
$$\delta = \frac{W_t - W_{t-\text{sphere}}}{W_{t-\text{sphere}}} \times 100\%.$$
(11)

For a specific non-spherical particle shape, δ remains essentially unchanged in the ¹³

Stokes regime, whereas δ decreases progressively with increasing Re_p in the 245 intermediate regime. Fig. 2 also shows that δ varies with particle shape. In addition to 246 the CSF, the aspect ratio obtained by dividing d_1 by d_s is selected here to account 247 for the shape effect. In the Stokes regime with low Re_p , δ is largely dependent on 248 249 aspect ratio, with larger particle aspect ratio corresponding to smaller terminal velocity. 250 The foregoing observations indicate that the longest and shortest form dimensions may 251 govern terminal velocity in the Stokes regime. Therefore, elongated, flat particles may reach almost equal values of terminal velocity despite their distinct shapes. When Re_p 252 253 exceeds 10, the computed δ generally decreases with decreasing CSF, and little 254 consistency is observed between δ and the aspect ratio. In short, when the viscous force 255 dominates, the terminal velocity is less affected by the non-spherical particle shape, which 256 can be characterized by the particle aspect ratio. When the inertial force becomes dominant, the shape effect tends to become significant, and should be represented by 257 258 CSF instead of aspect ratio.

Figure 3 illustrates the drag coefficient C_d as a function of particle Reynolds number Re_p . Results obtained from the spherical drag law proposed by Clift and Gauvin¹¹ are also included for comparison. The computed C_d curve for spheres exhibits satisfactory agreement with Clift and Gauvin's empirical relationship, confirming the validity of the present model. Non-spherical particles are predicted to experience relatively larger drag than equivalent spheres, with the difference between drag coefficient values progressively increasing as Re_p increases.

266 When a particle moves through a fluid, the total drag exerted on its surface can be 267 divided into pressure drag (or form drag) F_{pd} and friction drag F_{fd} . We consider the

drag ratio F_{fd}/F_{pd} which is defined as the ratio between friction drag and pressure drag 268 269 of a particle at the terminal settling state. Figure 4 illustrates the dependency of the drag ratio F_{fd} / F_{pd} on particle Reynolds number Re_p . The computed F_{fd} / F_{pd} of spheres 270 settling in the Stokes regime is approximately 2, close to the theoretically derived value.² 271 Moreover, the computed F_{fd} / F_{pd} of a specific shape remains constant throughout the 272 Stokes regime and gradually decreases as Re_p increases in the intermediate regime. For 273 given Re_p , the value of F_{fd}/F_{pd} generally increases with increasing CSF. These 274 275 results suggest that when the inertial force becomes significant or the particle shape 276 deviates from spherical, pressure drag gradually dominates over friction drag.



278

FIG. 1. Dimensionless terminal velocity W_{t*} against dimensionless spherical equivalent diameter d_* obtained for different particle shapes when $\beta_0 = 0^\circ$. Solid line refers to the model by Dietrich¹⁴.



FIG. 2. Predicted dependence of relative deviation δ in terminal velocity of a nonspherical particle to that of a sphere of the same equivalent diameter on particle Reynolds number Re_p .



FIG. 3. Dependence of predicted drag coefficient C_d on particle Reynolds number Re_p . Solid line is the spherical drag law proposed by Clift and Gauvin¹¹.

- 291
- 292



FIG. 4. Predicted dependence of drag ratio F_{fd} / F_{pd} on particle Reynolds number Re_p .

296 2. Characteristic time and displacement

Although the settling velocity and drag coefficient have been extensively studied for both spherical and non-spherical particles, limited attention has been paid to the time and space scales required for a particle to reach its terminal settling state.

The motion of a spherical particle falling through a fluid is described theoretically
by the Boussinesq-Basset-Oseen equation,² expressed as

302
$$\left(m_{p} + \alpha_{m}m_{f}\right)\frac{dW}{dt} = (m_{p} - m_{f})g - F_{d} - \frac{3}{2}d_{n}^{2}\left(\pi\rho_{f}\mu\right)^{1/2}\int_{0}^{t}\frac{dW}{d\sigma}\frac{d\sigma}{(t-\sigma)^{1/2}},$$
(12)

303 where m_f is the mass of fluid displaced by the sphere; α_m is the added mass coefficient; 304 and σ is a dummy variable. In Eq. (12), the term on the left-hand side denotes particle 305 inertia, and includes the added mass effect when an accelerating (or retarding) particle 306 moves in a fluid. In practice, it is common to assume $\alpha_m = 0.5$. On the right-hand side 307 of Eq. (12), the first term is the submerged weight of the particle, the second term 308 represents the fluid drag, and the third term is the Basset force (due to particle acceleration 309 because of unsteady viscous shear on the surface of the particle).

Guo⁴⁴ derived a simple closed-form solution for the motion of a sphere settling 310 through a fluid by applying Rubey's drag law⁴⁵ to Eq. (12) and combining the added mass 311 312 and the Basset force into an integrated term. Guo was able to determine analytically the 313 time-dependent settling velocity, acceleration, and vertical displacement of a spherical 314 particle. However, for a non-spherical particle, even when the orientation variation is 315 neglected and the drag force approximated by an empirical relationship, it is extremely 316 difficult to obtain analytical solutions for the added mass and the Basset force. In practice, 317 empirical relations have to be introduced in order to describe the characteristic time and 318 characteristic displacement of a settling non-spherical particle.

Here, we focus on cases with $\beta_0 = 0^\circ$, where particles accelerate to the terminal settling state with negligible change in orientation. The characteristic time t_{95} and characteristic displacement s_{95} are defined as the time and vertical displacement taken for a particle to reach 95% of its terminal velocity. A general dimensional analysis gives the following expressions:

324
$$t_{95*} = \frac{t_{95}}{d_n^2 / \nu} = f_1 \left(Re_p \right), \tag{13}$$

325
$$s_{95*} = \frac{s_{95}}{d_n} = f_2(Re_p), \qquad (14)$$

where t_{95*} and s_{95*} are dimensionless characteristic time and displacement. Figure 5 326 depicts the behavior of t_{95*} and s_{95*} with Re_p , as logarithmic plots. Linear fitting is 327 328 used to obtain two asymptotes for the Stokes and intermediate regimes, with their 329 intersection set at $Re_p = 1$. As shown in Fig. 5(a), the dimensionless characteristic time t_{95*} is assumed constant throughout much of the Stokes regime, and then decreases with 330 increasing Re_p in the intermediate regime. The dimensionless characteristic 331 displacement s_{95*} increases monotonically with increasing Re_p over the simulated 332 333 range, with the linear slope observed in the Stokes regime reducing in the intermediate 334 regime [Fig. 5(b)]. These results suggest that the Stokes and intermediate regimes are 335 characterized by two distinct acceleration mechanisms. Based on the two asymptotes, the logarithmic matching approach proposed by Guo⁴⁶ is used to establish the following 336 337 correlation formulae:

338
$$t_{95*} = 2.226 \left(1 + Re_p^{3.126}\right)^{-0.222},$$
 (15)

339
$$s_{95*} = 1.716 R e_p^{0.998} \left(1 + R e_p^{3.409} \right)^{-0.209}.$$
 (16)

340 The above correlations are evaluated using the coefficient of determination R^2 and 341 mean relative error MRE, which are defined as

342
$$\mathbf{R}^{2} = 1 - \frac{\sum_{k=1}^{N} (\eta_{k}^{cal} - \eta_{k}^{sim})^{2}}{\sum_{k=1}^{N} (\overline{\eta}^{sim} - \eta_{k}^{sim})^{2}}, \qquad (17)$$

343
$$MRE = \frac{1}{N} \sum_{k=1}^{N} \left| \frac{\eta_k^{cal} - \eta_k^{sim}}{\eta_k^{sim}} \right|, \qquad (18)$$

where η_k^{cal} is the *k*-th data value obtained from the correlation functions; η_k^{sim} is the *k*-344 th data value from the numerical simulations; $\overline{\eta^{\text{sim}}}$ is the mean value of the simulated 345 data; and N is the number of pairs of data points. In general, higher R^2 and lower 346 347 MRE correspond to better model performance. As demonstrated in Table III, our theoretical model exhibits rather good performance with high R^2 and acceptable 348 349 MRE. The proposed correlations indicate that the time and space scales required for a non-spherical particle to reach its terminal settling state may vary with Re_p , and provide 350 351 convenient methods that give effective estimates of the magnitudes of the characteristic 352 time and displacement. It should be noted that the proposed correlations are only valid within the simulated range of Re_p for a particle-to-fluid density ratio ρ_p / ρ_f of 2.65. 353 Future work will be extended to the Newton regime ($Re_p > 10^3$) and incorporate a larger 354 355 range of density ratios.

TABLE III. Performance of proposed correlation formulae Eq. (15) for dimensionless
 characteristic time and Eq. (16) for dimensionless characteristic displacement against
 underlying simulated data.

Correlation	\mathbf{R}^2	MRE (%)
Eq. (15)	0.9971	5.948
Eq. (16)	0.9988	3.453



FIG. 5. Dependence on particle Reynolds number Re_p of (a) dimensionless 363 characteristic time t_{95*} and (b) dimensionless characteristic displacement s_{95*} .

365 B. Particle settling for different initial orientations.

366 *1.* Stokes regime

In this section, results from numerical cases with $d_n = 0.0625 \text{ mm}$ and Re_p ranging from 0.1 to 0.2 are analyzed to investigate the effect of initial orientation on the settling of non-spherical particles in the Stokes regime. Note that similar results are found for cases with $d_n = 0.015625 \text{ mm}$ and $2 \times 10^{-3} < Re_p < 3 \times 10^{-3}$, and so are not included here.

372 Taking ellipsoid 1 as an example, Fig. 6 shows the temporal variations in orientation angle β , settling velocity W, and vertical displacement s. It can be seen that β 373 remains constant during the settling process for cases with different β_0 [Fig. 6(a)]. This 374 375 suggests that the orientation remains essentially unchanged for non-spherical particles settling in the Stokes regime, in agreement with previous findings.^{27,28} As a result, a non-376 377 spherical particle reaches a terminal velocity that depends on the initial orientation of the particle [Fig. 6(b)]. And particles with larger β_0 tend to settle faster, yielding longer 378 379 vertical displacements [Fig. 6(c)].

To account for the effect of particle orientation, we consider crosswise sphericity ϕ_c , which is the ratio between the cross-sectional area of a volume-equivalent sphere and the projection area of the actual particle perpendicular to the flow.¹⁶ According to the definition of β , particles with large β should have relatively small projection areas and consequently develop large ϕ_c .

Figure 7 illustrates the influence of particle orientation on terminal settling state by showing the resulting variations in terminal velocity W_t and drag ratio F_{fd} / F_{pd} with ϕ_c . In general, larger ϕ_c leads to larger W_t , indicating that the particle experiences

lower total drag at larger β . In addition, F_{fd}/F_{pd} tends to increase as ϕ_c increases, 388 389 implying that the contribution from friction drag may increase despite reduction in total 390 drag when the particle is oriented away from $\beta = 0^{\circ}$. Figure 8 presents contour plots of 391 vertical flow velocity in the vicinity of particles of different shapes and initial orientation $\beta_0 = 45^\circ$ at the terminal settling state. Cases with $\beta_0 = 45^\circ$ are of particular interest 392 393 because the particles display asymmetric forms in the vertical plane. As shown in Fig. 8, 394 the velocity contours exhibit a highly symmetric pattern and turn out to be similar for 395 different particle shapes. The particles seem to move in combination with the surrounding 396 fluid, and so the effect of asymmetry of the solid shape is marginal. Arguably, this 397 accounts for the sustainability of random orientations.



398

399 FIG. 6. Time histories of (a) orientation angle β , (b) settling velocity W, and (c)

400 vertical displacement *s* for ellipsoid 1 with $d_n = 0.0625 \text{ mm}$.



FIG. 7. Predicted dependencies of (a) terminal velocity W_t and (b) drag ratio F_{fd} / F_{pd} 404 on crosswise sphericity ϕ_c for particles of different shapes with $d_n = 0.0625$ mm.



407 **FIG. 8**. Contour plots of vertical flow velocity around differently shaped particles with 408 $d_n = 0.0625 \text{ mm}$ and $\beta_0 = 45^\circ$ at the terminal settling state (t = 0.06 s): (a) ellipsoid 1, 409 (b) ellipsoid 2, (c) cylinder, and (d) disk.

411 *2. Intermediate regime*

Here numerical cases with $d_n = 1 \text{ mm}$ and $Re_p \approx 100$ are selected to probe into 412 413 the effect of initial orientation on the settling of non-spherical particles in the intermediate 414 regime. As can be seen from Fig. 9(a), particles of ellipsoid 1 shape tend to attain the 415 same terminal settling state with $\beta = 0^{\circ}$ irrespective of their initial orientation, consistent with the previously mentioned settling behavior at relatively large Re_{p} .^{8,29} 416 417 Variation in particle orientation has a vital effect on the settling process, about which more 418 details are given later in this section. Yet, due to the identical orientation attained at 419 terminal settling, the effect of initial orientation on terminal velocity can be negligible 420 [see Fig. 9(b)]. Except for the disk, similar results have been found for other particle shapes. At the terminal settling state, periodic oscillations about $\beta = 0^{\circ}$ are observed 421 for the disk particle [Figs. 9(d) and 9(e)]. Such results are in accordance with previous 422 observations by Stringham et al.⁴⁷ at a higher value of Re_p . 423

424 Fig. 10 depicts two-dimensional visualizations of the settling trajectory and orientation variation of different particles with $\beta_0 = 90^\circ$. The red dashed line denotes the 425 426 centroid trajectory and the black solid line with blue endpoints denotes the location of the 427 revolution axis. The time increment between each visualization is 0.02 s. During the 428 settling process, the revolution axes of elongated particles (ellipsoid 1 and the cylinder) 429 become gradually oriented normal to the direction of settling motion, while those of flat 430 particles (ellipsoid 2 and the disk) turn to be parallel to the settling direction, thus the 431 $\beta = 0^{\circ}$ state is eventually reached. In addition to the vertical fall, a horizontal component 432 can be observed in the settling path, associated with the varying orientation.



FIG. 9. Time histories of orientation angle β , settling velocity W, and vertical 436 displacement *s* for (a-c) ellipsoid 1 and (d-f) disk with $d_n = 1 \text{ mm}$.



438

439 **FIG. 10**. Variations in settling trajectory and orientation of different particles with 440 $d_n = 1 \text{ mm}$, $\beta_0 = 90^\circ$ and shape: (a) ellipsoid 1, (b) ellipsoid 2, (c) cylinder, and (d) disk. 441 Red dashed line denotes the centroid trajectory, and black solid line with blue endpoints 442 denotes the location of the revolution axis. The lengths of the revolution axes of ellipsoid 443 2 and the disk are doubled and tripled respectively for clarity. The time increment between 444 each visualization is 0.02 s.

445 Given that gravitational force induces no torque about the mass center, torque arising 446 from hydrodynamic forces is responsible for particle rotation. According to Mandø and 447 Rosendahl⁸, friction torque always acts to damp rotational motion, whereas torque 448 stemming from the offset of the center of pressure from the geometric center (i.e., the 449 mass center) accounts for particle readjustment. Figure 11 illustrates the pressure distribution around ellipsoid 1 at different instants of settling for $\beta_0 = 90^\circ$. During the 450 initial period, the particle moves at its initial orientation (i.e., $\beta = \beta_0 = 90^\circ$) [Fig. 11(a)]. 451 452 Although the particle experiences no torque under such circumstances, this can 453 instinctively be interpreted as a state of unstable equilibrium. Once it experiences a certain 454 level of disturbance, the particle starts to deviate from the state of unstable equilibrium, 455 and the pressure distribution is no longer symmetric around the particle [Figs. 11(b) and 456 11(c)]. This change promotes additional torque due to the displacement of the center of 457 pressure, thus forcing the particle to rotate. Eventually, a state of stable equilibrium is 458 reached whereby the center of pressure is consistent with the geometric center, and the 459 torque vanishes [Fig. 11(d)]. The terminal settling state of a particle is commonly 460 characterized by this stable equilibrium state without regard to secondary motions like 461 oscillation.

Based on the above description, the settling process of a non-spherical particle in the intermediate regime may be divided into three chronological stages. In Stage 1, the particle provisionally settles at an unstable equilibrium state. In Stage 2, the particle selfreadjusts to the stable equilibrium state. In Stage 3, the particle progressively attains the terminal settling state where secondary motions may occur. Notably, particles with certain initial orientations may not experience Stage 1 and even Stage 2. Moreover, the settling velocity can dramatically increase in Stage 1, leading to a considerably longer vertical 469 displacement [see Figs. 9(c) and 9(f)]. Particles with $d_n = 0.25 \text{ mm}$ ($Re_p \approx 10$) exhibit 470 qualitatively similar settling behavior to those with $d_n = 1 \text{ mm}$, yet appear to be oriented 471 directly to the stable equilibrium state of $\beta = 0^\circ$ without exhibiting oscillations in Stage 472 2 (Fig. 12).

473 As a settling particle rotates due to hydrodynamic torque, the rotational motion of 474 the particle can in turn appreciably affect the flow field around it and may thus promote 475 specific wake structures. Fig. 13 visualizes the flow fields around particles of different shapes with $d_n = 1 \text{ mm}$ and $\beta_0 = 90^\circ$. The Ω_R method proposed by Dong et al.⁴⁸ is 476 used for vortex identification. An iso-surface of $\Omega_R = 0.52$ is chosen to capture the 477 478 vortical structures. As illustrated in Fig. 13(a), the wake of ellipsoid 1 initially consists of 479 two thread-like vortices that are attached to the particle. As the particle rotates, instability 480 develops, and vortex shedding occurs. The detaching vortices push the flow near and 481 around the particle upwards, forming a low-pressure region that generates a torque on the 482 particle in the opposite direction. This additional torque along with inertia can further lead 483 to particle oscillations because new vortices can detach on the other side when the particle 484 reaches the opposite inclination and so on, each time it changes orientation. Notably, the 485 vortical structure is closely related to the particle shape. Similar to ellipsoid 1, a double-486 threaded wake structure is observed for the cylinder [Fig. 13(c)], whereas flatter particles like ellipsoid 2 and the disk present a so-called hairpin structure^{49,50} [Figs. 13(b) and 487 13(d)]. Vortex shedding is less pronounced for particles with $d_n = 1 \text{ mm}$ and $\beta_0 = 45^\circ$. 488 This is mainly because the absence of Stage 1 leads to relatively low Re_p in Stage 2. 489 For particles with $d_n = 0.25$ mm however, no vortex shedding is observed for all 490 491 simulated shapes and initial orientations. The foregoing suggests that the occurrence of 492 vortex shedding depends largely on the magnitude of Re_p . An unstable initial orientation 493 may promote vortex shedding because larger Re_p can be reached and rotational motion 494 is induced. In turn, vortex shedding can affect the settling motion by causing the particle 495 to oscillate in Stage 2 and Stage 3.

Figure 14 presents contour plots of the vertical flow velocity component around particles of different shapes for $d_n = 1 \text{ mm}$ and $\beta_0 = 90^\circ$. Sinuous wake structures associated with varying particle orientation can be observed. Moreover, the velocity distribution in the wake exhibits an asymmetric pattern even as the particle approaches the state of stable equilibrium [Figs. 14(a) and 14(d)]. In fact, the high-velocity zone is located close to the downward-rotating end of the particle, reflecting the effect of rotational motion on the flow field.

503 Overall, our results provide insight into the settling process of non-spherical particles 504 in the intermediate regime. The initial orientation of non-spherical particles plays a key 505 role in the settling process and so should be taken into account for particulate flows.



508 **FIG. 11.** Pressure distribution contours around ellipsoid 1 with $d_n = 1 \text{ mm}$ and 509 $\beta_0 = 90^\circ$ at different instants of settling: t = (a) 0.04 s, (b) 0.10 s, (c) 0.14 s, and (d) 510 0.60 s.



FIG. 12. Time histories of (a) orientation angle β , (b) settling velocity W, and (c) 514 vertical displacement *s* for ellipsoid 1 with $d_n = 0.25$ mm.



516

517 **FIG. 13.** Vortices in the wake of particles of different shapes for $d_n = 1 \text{ mm}$ and 518 $\beta_0 = 90^\circ$ during orientation readjustment: (a) ellipsoid 1, $t = 0.12 \sim 0.22$ s, (b) ellipsoid 2, 519 t = 0.18 s, (c) cylinder, t = 0.20 s, and (d) disk, t = 0.30 s. An iso-surface of $\Omega_R = 0.52$ 520 is chosen to capture vortical structures.⁴⁸



FIG. 14. Contour plots of vertical flow velocity component around particles of different shapes with $d_n = 1 \text{ mm}$ and $\beta_0 = 90^\circ$ during orientation readjustment: (a) ellipsoid 1, t = 0.22 s, (b) ellipsoid 2, t = 0.18 s, (c) cylinder, t = 0.20 s, and (d) disk, t = 0.30 s.

527 IV. CONCLUSION

528 This study has investigated the effects of particle shape and initial orientation on the 529 settling of non-spherical particles. Commercial CFD software FLOW-3D was used to 530 perform a series of PR-DNS simulations of the settling in otherwise quiescent water of 531 spheres and five types of regular, non-spherical sediment particles, i.e., prolate spheroid, 532 oblate spheroid, cylinder, disk, and cube. A dual-Euler whole-attitude solver was used to 533 reproduce particle orientation behavior. In the study, the Galileo number was varied from 534 0.248 to 360 with the particle Reynolds number Re_p ranging from 0.00277 to 562. 535 Based on the computational results, the main findings are summarized as follows: 536 (1) A non-spherical particle experiences larger drag and consequently attains a lower

terminal velocity than its spherical counterpart. For sufficiently small Re_p when the viscous force dominates, the terminal velocity is less affected by the particle shape (characterized by the particle aspect ratio). For relatively large Re_p when the inertial force becomes dominant, the shape effect becomes significant, and should be represented by the Corey shape factor. When the inertial force becomes significant or the particle shape deviates from a sphere, then pressure drag may dominate over friction drag.

544 (2) Empirical correlations were derived for the dimensionless characteristic time 545 t_{95*} and dimensionless characteristic displacement s_{95*} of particle settling. It 546 was demonstrated that t_{95*} remains constant in the Stokes regime and decreases 547 as Re_p increases in the intermediate regime; s_{95*} increases logarithmically 548 with increasing Re_p over the simulated range, whereas the slope in s_{95*} with

 Re_n observed in the Stokes regime reduces in the intermediate regime.

(3) In the Stokes regime, the orientation of a non-spherical particle remains essentially unchanged during the settling process. A non-spherical particle with different initial orientations can attain various terminal velocities which increase with crosswise sphericity ϕ_c . The flow velocity distribution in the vicinity of a particle of any shape exhibits a highly symmetric pattern. A given particle appears to move in tandem with the surrounding fluid, such that the effect of its asymmetry is marginal.

557 (4) In the intermediate regime, a non-spherical particle provisionally settling at an 558 unstable orientation tends to readjust itself to a stable equilibrium state. In 559 general, such a particle may experience three stages during its settling process: 560 settling provisionally at an unstable equilibrium state; self-readjusting to the 561 stable equilibrium state; and progressively approaching the terminal state where 562 secondary motions may occur. Due to the identical orientation attained at 563 terminal settling, the effect of initial orientation on terminal velocity is negligible, 564 while an unstable initial orientation can result in a longer vertical displacement 565 and may promote vortex shedding. It is therefore important to consider the initial 566 orientation of non-spherical particles when modeling particulate flows.

In many real-world situations, particles do not settle in isolation. Vortices induced by nearby particles can significantly influence the overall settling behavior, e.g., causing repulsion in dual-particle cases,⁵¹ promoting clusters for monodisperse particles,⁵² and altering the orientation of rod-like particles.⁵³ Direct inter-particle interactions (collisions) also play an important role in the dynamics of particles particularly when in a dense regime.^{54,55} Therefore, we intend to carry out future research into the behavior of multi-

- 573 particle systems. Moreover, the present work has provided us with a unique basis to
- 574 investigate the settling of irregular particles; this work is underway.
- 575

576 SUPPLEMENTARY MATERIAL

- 577 The Supplementary Material provides a brief description of the dual-Euler whole-578 attitude solver used to model variation in particle orientation.
- 579

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584 AUTHOR DECLARATIONS

- 585 Conflict of Interest
- 586 The authors have no conflicts to disclose.
- 587

588 Author Contributions

589 Xiaoyong Cheng: Data curation (lead); Formal analysis (lead); Investigation (equal);

- 590 Methodology (equal); Validation (lead); Visualization (lead); Writing original draft
- 591 (lead). Zhixian Cao: Conceptualization (equal); Funding acquisition (lead); Investigation
- 592 (equal); Methodology (equal); Project administration (lead); Resources (lead);

593	Supervision (lead); Writing – review & editing (equal). Ji Li: Conceptualization (equal);
594	Investigation (equal); Writing - review & editing (equal). Alistair Borthwick:
595	Conceptualization (equal); Investigation (equal); Writing - review & editing (equal).
596	

597 DATA AVAILABILITY

598 Data that support the findings of this study are available from the corresponding 599 author upon reasonable request.

600

601 APPENDIX: VALIDATION OF THE CFD MODEL

602 The settling of a solid sphere in quiescent water was experimentally investigated by Mordant and Pinton⁵⁶ who derived the temporal variation in settling velocity from 603 604 measurements of the Doppler shift of an ultrasonic wave scattered by a moving particle. 605 Two cases with $d_n = 0.5 \text{ mm}$ and 1.5 mm are simulated to validate the applied CFD model. The particle density is $\rho_p = 2560 \text{ kg/m}^3$, the water density is $\rho_f = 1000 \text{ kg/m}^3$, 606 and the dynamic viscosity of water $\mu = 8.9 \times 10^{-4}$ kg/m/s. The simulation setup is the 607 608 same as previously described in Sec. II.B except that three mesh resolutions are tested, 609 i.e., $\Delta h = 1/10$, 1/12, and $1/14 d_n$.

610 Fig. 15 shows that there is good agreement between the simulated and measured 611 settling velocities, thus validating the model, and demonstrating that a mesh resolution of 612 $\Delta h = 1/12d_n$ is sufficiently fine to produce accurate results.



615 **FIG. 15.** Time history of settling velocity W for spheres of (a) $d_n = 0.5$ mm and (b) 616 $d_n = 1.5$ mm. Black solid line refers to measured data by Mordant and Pinton⁵⁶. 617

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