Collision rates of small ellipsoids settling in turbulence

Citation for published version (APA):

DOI:
10.1017/jfm.2014.554

Document status and date:
Published: 01/01/2014

Document Version:
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher’s website.
• The final author version and the galley proof are versions of the publication after peer review.
• The final published version features the final layout of the paper including the volume, issue and page numbers.

Link to publication

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
• You may not further distribute the material or use it for any profit-making activity or commercial gain
• You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the “Taverne” license above, please follow below link for the End User Agreement:
www.tue.nl/taverne

Take down policy
If you believe that this document breaches copyright please contact us at:
openaccess@tue.nl
providing details and we will investigate your claim.
Collision rates of small ellipsoids settling in turbulence

C. Siewert¹,†, R. P. J. Kunnen² and W. Schröder¹

¹Institute of Aerodynamics, RWTH Aachen University, Wüllnerstrasse 5a, 52062 Aachen, Germany
²Fluid Dynamics Laboratory, Department of Physics and J.M. Burgers Centre for Fluid Mechanics, Eindhoven University of Technology, PO Box 513, 5600 MB Eindhoven, The Netherlands

(Received 17 March 2014; revised 7 August 2014; accepted 18 September 2014; first published online 10 October 2014)

We propose that the collision rates of non-spherical particles settling in a turbulent environment are significantly higher than those of spherical particles of the same mass and volume. The theoretical argument is based on the dependence of the particle drag force on the particle orientation, thus varying gravitational settling velocities, which can remain different until contact due to the particle inertia. Therefore, non-spherical particles can collide with large relative velocities. Direct numerical simulations (DNS) of streamwise decaying isotropic turbulence seeded with small, heavy, rotationally symmetric ellipsoids of five different aspect ratios are performed to confirm these arguments. The motion of 21 million ellipsoids is tracked by a Lagrangian particle solver assuming creeping flow conditions and neglecting the influence of the particles on the flow. We find that ellipsoids collide considerably more often than spherical particles of the same volume and mass due to a drastically increased mean relative velocity at contact.

Key words: isotropic turbulence, multiphase and particle-laden flows, turbulence simulation

1. Introduction

Collisions of small, heavy, non-spherical particles settling in turbulent flows occur frequently in nature and industry, like, for example, ice crystals in clouds (Pruppacher & Klett 1997), dust in protoplanetary disks (Williams & Cieza 2011), or fibres in papermaking (Lundell, Söderberg & Alfredsson 2011). Particle growth in such systems proceeds through collisions: two colliding particles can stick together. The collision rate is thus a measure of particle growth. Despite this importance of small, heavy, non-spherical particles, knowledge about their collisions in turbulence is very limited since they are extremely hard to investigate experimentally and numerically.

During the last two decades the collision rates of heavy spherical particles have been the subject of many, mostly numerical studies (e.g. Bec et al. 2005; Wang et al. 2008) that have revealed the complex dynamic interactions of inertial particles with gravity and turbulence. However, non-spherical particles in turbulence are hardly considered in the literature. Recently, the motion of neutrally buoyant non-spherical particles has been focused on (e.g. Pumir & Wilkinson 2011; Parsa et al. 2012)

† Email address for correspondence: c.siewert@aia.rwth-aachen.de
Collision rates of small ellipsoids settling in turbulence

Figure 1. Sketches of identical heavy particles settling due to gravity $g$ (see § 1). In quiescent conditions spherical particles do not settle differently ($a$). The same is valid for non-spherical particles ($b$). In mild turbulence spheres can have relative velocities although the gravitation-induced velocity is the same and does not contribute to the relative velocity ($c$). In contrast non-spherical particles might become differently oriented by turbulent eddies such that the resulting different settling velocities lead to significant relative velocities ($d$).

revealing the interesting coupling of their rotational motion with the fluid velocity gradient tensor. Investigations of heavy non-spherical particles in turbulence focus on the motion and deposition of prolate ellipsoids in channel flow (Bernstein & Shapiro 1994; Zhang et al. 2001; Mortensen et al. 2008; Marchioli, Fantoni & Soldati 2010). Recently, we have investigated the motion of both oblate and prolate ellipsoids in isotropic decaying turbulence by direct numerical simulations (DNS) and found that depending on the turbulence intensity the ellipsoids preferentially sample the downward-moving sides of the turbulent eddies, leading to faster settling compared to quiescent flow conditions and to an alignment of the longest ellipsoid axis with the direction of gravity (Siewert et al. 2014b). We hypothesized that both effects might influence the collision probabilities of the ellipsoids.

Two identical heavy spheres settle with equal velocities in quiescent conditions, hence a collision is very unlikely, see figure 1($a$). However, in turbulence the collision likelihood is different (figure 1$c$). For particle relaxation time scales in the range of the turbulent time scales, the particles are driven out of turbulent eddies and cluster outside (Squires & Eaton 1991; Wang & Maxey 1993; Sundaram & Collins 1997; Saw et al. 2012). This increases the number of possible collision partners but due to the spatial correlation the relative velocity of the collision partners is rather small. If the particle time scale is large the motion is more ballistic. Hence, if two particles are accelerated by different vortices they can reach the same point in space and time but at different velocities (Abrahamson 1975; Falkovich, Fouxon & Stepanov 2002; Wilkinson, Mehlig & Bezuglyy 2006; Falkovich & Pumir 2007; Bec et al. 2010). This so-called sling effect has recently been observed in experiments (Bewley, Saw & Bodenschatz 2013).
In quiescent conditions, non-spherical particles will also settle with equal velocities, although their settling velocities are smaller compared to spheres of the same mass (figure 1b). However, in turbulence non-spherical particles might come into contact at large relative velocities simply because they feature different orientations due to the orientation-dependent drag force. If one of two initially equally oriented particles is rotated by a turbulent eddy, its settling direction and velocity change, see figure 1(d). Thus, it is possible that two non-spherical particles arrive simultaneously at the same point with a large relative velocity. The question to be addressed is: how likely are two particles at different orientations to be at the same point in a turbulent fluid?

To the best of our knowledge we are the first to consider the collision rates of ellipsoidal particles settling in turbulence. It will be shown, first theoretically (see § 2), and then by numerical simulations (see § 3), that both prolate and oblate ellipsoids are more likely to collide than spheres of the same volume and mass. We summarize our findings in § 4.

2. Theory

2.1. Particle model

To answer the question of the likelihood of unaligned collisions, we first consider the problem theoretically based on the following particle model. Afterwards, we conduct a numerical experiment with the same particle model.

The particles considered are much smaller than the Kolmogorov length scale $\eta_k$ and much heavier than the fluid. As a result the particle Reynolds number $Re_p < 1$ and the fluid forces and torques on the particles can be approximated assuming creeping flow conditions. The fluid forces and torques are known analytically for rotationally symmetric ellipsoids (Happel & Brenner 1965), which are characterized by their aspect ratio $\beta$ relating the principal semi-axes $a = b = c/\beta$. These ellipsoids are commonly used as a first-order approximation to general non-spherical particles. For instance, the two fundamental types of ice crystals in clouds, i.e. prismatic hexagonal columns and disks, are well approximated by rotationally symmetric ellipsoids (Pruppacher & Klett 1997). The ellipsoid orientation can be tracked by the rotation between the inertial coordinate system ($x, y, z$) and a particle-fixed coordinate system ($\hat{x}, \hat{y}, \hat{z}$). This frame of reference is fixed at the particle centre of mass and rotates with the particle such that the ellipsoidal symmetry axis $c$ is always aligned with the $\hat{z}$ direction. The corresponding rotation matrix $A$ can be composed of the Euler angles $\theta, \phi, \psi$ for presentation purposes (see figure 2) or of quaternions for simulations due to their numerical superiority (Fan & Ahmadi 1995).

In the Stokes limit, the particle linear acceleration depends only on the gravity $g$ and the hydrodynamic drag force (Oberbeck 1876)

$$\frac{dv}{dr} = g + \frac{24}{9} \frac{\beta^{2/3}}{\tau_p} A^{-1} \begin{pmatrix} \frac{1}{\chi_0/a^2 + \alpha_0} & 0 & 0 \\ 0 & \frac{1}{\chi_0/a^2 + \alpha_0} & 0 \\ 0 & 0 & \frac{1}{\chi_0/a^2 + \beta^2 \gamma_0} \end{pmatrix} A(u - v), \quad (2.1)$$

where the latter is linearly proportional to the difference between the particle velocity $v$ and fluid velocity $u$ at the particle position. The quantity $\tau_p = 2 \rho_p r^2/(9 \rho_f v)$ is the particle response time of a sphere of radius $r$ with the same volume and mass as the
ellipsoid, depending on the particle density \( \rho_p \), the fluid density \( \rho_f \), and the kinematic viscosity \( v \). The shape factors \( \alpha_0, \gamma_0 \), and \( \chi_0 \) are functions of the aspect ratio \( \beta \), see table 1. For \( \beta = 1 \) the drag tensor becomes isotropic since \( \alpha_0 = \gamma_0 \), the rotation matrix \( A \) has no effect, and the equation is reduced to the simplified Maxey–Riley equation commonly used for spherical particles in turbulence (e.g. Bec et al. 2006; Wang et al. 2008). The particle angular velocity \( \omega \) in the particle-fixed coordinate system does not depend on gravity but on the hydrodynamic torque (Jeffery 1922)

\[
\begin{align*}
\frac{d\omega_z}{dt} & = \frac{\omega_x \omega_z \beta^2 - 1}{1 + \beta^2} + \frac{40 \beta^{2/3}}{9} \frac{\tau_{p}}{\tau_{f}} \left( \frac{1}{\alpha_0 + \beta^2 \gamma_0} \right) \\
\frac{d\omega_y}{dt} & = \frac{\omega_x \omega_z \beta^2 - 1}{1 + \beta^2} + \frac{40 \beta^{2/3}}{9} \frac{\tau_{p}}{\tau_{f}} \left( \frac{1}{\alpha_0 + \beta^2 \gamma_0} \right) \\
\frac{d\omega_x}{dt} & = \frac{1}{1 + \beta^2 \tau_{z\theta}} \left( \frac{\tau_{z\theta} - \omega_x}{1 + \beta^2 \tau_{z\theta}} \right) + \left( \frac{\tau_{z\phi} - \omega_y}{1 + \beta^2 \tau_{z\phi}} \right),
\end{align*}
\]

where \( \tau_{ij} = (\partial u_i / \partial x_j + \partial u_j / \partial x_i) / 2 \) denotes the fluid shear stress and \( \xi_{ij} = (\partial u_i / \partial x_j - \partial u_j / \partial x_i) / 2 \) the vorticity.

This particle model is only valid for \( Re_p = 0 \). Using perturbation methods Brenner & Cox (1963) showed for arbitrarily shaped particles that additional forces and moments arise with increasing particle Reynolds number. While the corrections for the translational motion are only of higher order, the corrections might be important for the rotational degree of freedom (Leal 1980). For intermediate particle Reynolds numbers, particles are known to settle with their broad side horizontally in a quiescent atmosphere (Feng, Hu & Joseph 1994; Newsom & Bruce 1994). For weak fluid inertia, Cox (1965) showed using perturbation methods that the orientating torque scales linearly with the particle Reynolds number for a nearly spherical particle. In the opposite limit of very large aspect ratios, Shin, Koch & Subramanian (2006) showed the same dependence on the Reynolds number using slender body theory. However, to the authors’ knowledge a general nonlinear correction has not been obtained in
the literature to date, not even for ellipsoids (Chester 1990). Hence, although (2.1) and (2.2) are only leading-order approximations for inertial ellipsoids they are still commonly used for particles in turbulent channel flows (Zhang et al. 2001; Mortensen et al. 2008; Marchioli et al. 2010). Recent results from particle resolving simulations of inertial particles at low Reynolds numbers support this usage of the Stokes torque for investigations of heavy particles (Mao & Alexeev 2014). Nevertheless, the limit of the approximation has to be kept in mind, especially if larger or heavier ellipsoids are analysed which can have significant particle Reynolds numbers.

2.2. Collision kernel

In meteorology and astrophysics the collision probability is typically used in the form of the collision kernel to investigate the evolution of particle size spectra (Dullemond & Dominik 2005; Xue, Wang & Grabowski 2008). For spherical particles there are two equivalent approaches to determine the collision kernel: the so-called kinematic and dynamic kernel (Wang, Wexler & Zhou 2000). Dividing the rate of collisions per unit volume $\dot{N}$ by the number of possible pairs of particles with concentration $n$, the dynamic collision kernel $\Gamma^D$ is obtained as

$$\Gamma^D = \dot{N} \frac{2}{n(n-1)}. \quad (2.3)$$

The equivalent kinematic collision kernel $\Gamma^K$ for spheres is given by

$$\Gamma^K = 2\pi(r_1 + r_2)^2 \langle |w_r (r_1 + r_2)| \rangle g_{11} (r_1 + r_2), \quad (2.4)$$

where $r_1 = r_2$ are the equal (collision) radii of the spheres, $\langle |w_r (r_1 + r_2)| \rangle$ is the mean radial relative velocity (RRV) at contact (Saffman & Turner 1956), and $g_{11} (r_1 + r_2)$ is the radial distribution function (RDF) at contact (Sundaram & Collins 1997). The kinematic description has the advantage that it includes information on how turbulence alters the collision mechanism (see § 1). For example, by increasing the tendency of the particles to cluster in specific regions of the flow the value of the RDF is increased. Likewise, turbulence can increase the RRV which enhances the collision rate.
In the following, a simple model as a first attempt at a theoretical estimate for the ellipsoidal collision kernel is discussed. Since we know that turbulence tends to randomize the particle orientation distribution function (Siewert et al. 2014b), we assume uncorrelated random orientations of the ellipsoids. Furthermore, we conjecture that the gravitation-induced relative settling dominates over the influence of the turbulent fluctuations such that settling can be considered in a quiescent environment \((u = 0)\). Under these assumptions, the ellipsoids will settle while staying in their initial random orientation (see (2.2)). The validity of the assumptions will be re-examined in the Results section, § 3.3.

In general, the settling velocity of a spheroid at a fixed orientation in a stagnant fluid \((u = 0)\), i.e. the solution of (2.1) by balancing gravity and drag force for fixed rotation angles \(\phi, \theta, \gamma\), can be written as

\[
v_t = \frac{9}{24} \left( \beta^2 \gamma_0 - \alpha_0 \right) \left( \begin{array}{c}
\cos \theta \sin \theta \sin \phi \\
- \cos \theta \sin \theta \cos \phi \\
\cos^2 \theta + \frac{\chi_0 a^{-2} + \alpha_0}{\beta^2 \gamma_0 - \alpha_0}
\end{array} \right) \frac{\tau_p}{\beta^{2/3}} g.
\] (2.5)

Without loss of generality, the \(z\) coordinate is chosen to point in the direction of gravity. It can be seen that the settling velocity is independent of \(\psi\) due to the rotational symmetry of the ellipsoids. In general, settling ellipsoids also exhibit a drift, i.e. they fall in an intermediate direction between the direction of gravity and the direction of their symmetry axis.

The ellipsoids will collide with random orientations, but for simplicity we assume contact at a constant distance of \(R_{12} = r_1 + r_2\) such that the RRV can be computed as the rate of volume influx through the surface of that collision sphere (Wang et al. 2000). Using the incompressibility of the volume inflow, i.e. the periodicity of the inflow with respect to the spherical coordinate system of the collision sphere, \(\langle |w_t(R_{12})| \rangle\) can be obtained by considering only the upper hemisphere of the collision sphere

\[
\langle |w_t(R_{12})| \rangle = \frac{1}{2 \pi R_{12}^2} \int_0^{2\pi} \int_0^{\pi/2} \left| (v_1 - v_2) \cdot \frac{x_1 - x_2}{\|x_1 - x_2\|} \right| R_{12} \sin \theta \, d\theta \, d\phi, \quad (2.6)
\]

with \(\theta\) the polar angle and \(\phi\) the azimuthal angle of the spherical coordinate system. Performing the surface integral for randomly oriented settling ellipsoids at contact, i.e. with \(\|x_1 - x_2\| = R_{12}, \quad (x_1 - x_2)/\|x_1 - x_2\| = (\sin \theta_c \cos \phi_c, \sin \theta_c \sin \phi_c, \cos \theta_c)^T\), and \(v = v_t(\theta, \phi)\) and averaging over all possible orientations at contact, leads to

\[
\langle |w_t(r_1 + r_2)| \rangle = \frac{3 \pi^2}{256} \tau_p g \beta^{-2/3} |\gamma_0 \beta^2 - \alpha_0| = \frac{3 \pi^2}{256} \tau_p g f(\beta). \quad (2.7)
\]

Although the drift velocity due to the ellipsoidal particle shape is accounted for, a collision sphere of a constant size is assumed; hence (2.7) is not fully correct. However, we have shown with simulations (Siewert et al. 2014a) that the approximation gives quantitatively reasonable results. In figure 3 the shape-dependent part \(f(\beta)\) of the RRV is plotted as a function of the aspect ratio. The gravitation-induced mean RRV is zero for spheres \((\beta = 1)\) of equal mass and volume since they settle at the same velocity in the direction of gravity (compare § 1 and (2.5)). However, the RRV is quite sensitive to \(\beta\) around \(\beta = 1\). At both small and large values of \(\beta\) the dependence levels off.
3. Numerical simulation

3.1. Numerical set-up

In order to show the validity of the concept indicated above we determine collision
statistics based on a numerical experiment on streamwise decaying turbulent flow
(Kunnen et al. 2013) with small heavy non-spherical particles in suspension (Siewert
et al. 2014b). The set-up is designed for water or ice at cloud conditions (Pruppacher
& Klett 1997). However, the results might also be directly applicable to dust in
protoplanetary disks (Williams & Cieza 2011) and cellular fibres in the paper-making
process (Lundell et al. 2011).

The turbulent air flow at a constant mean velocity \( \langle u \rangle \) through a vertically elongated
box of length \( L \) is simulated by solving the Navier–Stokes equations on an equidistant
Cartesian grid with a general purpose finite-volume solver (Hartmann, Meinke &
The mesh of approximately 53 million cells ensures a sufficient resolution for a
DNS at a Reynolds number \( Re_L = \langle u \rangle L / v = 8 \times 10^4 \). At the inflow the turbulence
is created by a method described in Batten, Goldberg & Chakravarthy (2004). Due
to viscous damping the turbulence decays in the streamwise direction and mimics
grid-generated wind tunnel turbulence. Kunnen et al. (2013) have shown that this
set-up is an equivalent alternative to the generic periodic cubic domain commonly
used for numerical investigations of particles in turbulence (e.g. Bec et al. 2006;
Wang et al. 2008).

Five types of ellipsoids are considered with \( \beta \) ranging from 0.25 to 4 but at
constant mass and volume, namely that of a sphere with radius \( r = 0.0435\eta_k \). The
particle density is 843 times larger than that of the fluid. Hence, the use of the Stokes
flow particle model (§ 2.1) can be justified by \( Re_p < 1 \). The particle concentration
expressed as the volume loading \( \Phi \) is very low, i.e. \( \Phi \approx 10^{-5} \), such that one-way
coupling between the flow and the particles can be assumed. That is the fluid
forces and torques influence the motion of the ellipsoids, but the influence of the
ellipsoids on the flow is neglected. Additionally, for the simplicity of this first study
the hydrodynamic interaction of the approaching particles is neglected. Hence, only
geometric collision probabilities (Devenish et al. 2012; Grabowski & Wang 2013) are

\[ f(\beta) = \sqrt{2 \Theta \beta^4 - a_0 \beta^{-3}} \]
Collision rates of small ellipsoids settling in turbulence

considered and the turbulence effects on the collision efficiency, which account for the hydrodynamic interaction effects on the collision probabilities (Pinsky, Khain & Shapiro 2007; Wang et al. 2008), are not investigated. A discussion of the impact of this simplification is given at the end of the Results section, § 3.3.

The ellipsoids are released randomly at the inflow plane and are transported through the decaying turbulence field by the constant mean flow velocity. Ellipsoids that leave the domain are reintroduced at the inflow plane to attain a statistically steady state. Downstream of the inflow plane, when the orientations and fluctuation velocities of the ellipsoids are independent of the initial release conditions, collision statistics are collected in a volume of small streamwise extent with a Reynolds number based on the Taylor scale of $R_{\lambda} = 20.5$ and a turbulent Froude number $Fr = \frac{\varepsilon^{3/8} g^{-1/2} v^{-1/8}}{\nu^{1/8}} = 0.265$ with $\varepsilon$ the mean turbulent kinetic energy dissipation rate. Due to the small particle sizes and time scales, their motion is mainly governed by the dissipation range of the fluid (Wang & Maxey 1993) such that the results are non-dimensionalized by the Kolmogorov scales. However, a Reynolds number dependence due to the lack of scale separation and turbulent intermittency is also expected (Grabowski & Wang 2013).

3.2. Collision detection

The collision kernel definitions in (2.3) and (2.4) are for spherical particles. The evaluation for non-spherical particles is quite challenging. There is no closed analytical formula to determine whether two arbitrarily oriented ellipsoids overlap (Zheng, Iglesias & Palffy-Muhoray 2009). Hence, for the determination of the dynamic kernel (2.3), which amounts to counting collisions per time interval, we have to use an iterative approach for the collision detection. We have compared and validated different methods for ellipsoidal collision detection in Siewert et al. (2014a). Based on this, the continuous collision detection method by Choi et al. (2009) is used in this study.

The kinematic kernel $\Gamma^K$ (2.4) is typically calculated by determining the individual contributions from nearby particles over many snapshots (Wang et al. 2000). For ellipsoids, this relation is formally a function of the orientation of the two touching ellipsoids. To fully resolve this angular dependence requires a vast amount of data and long-time averaging. Instead of attempting to gather enough statistics for an orientation-dependent form of $\Gamma^K$, the spherical kinematic kernel is used as stated in (2.4) to gain additional insight into how turbulence affects the collision mechanism of ellipsoids. Three radii are included to determine whether the ellipsoids are in contact. The correct value for the ellipsoidal collision kernel is bounded by the collision kernels evaluated at the edge of inscribed or bounding spheres with radii equal to the smallest ($r_{\text{min}} = \min(a, c)$) and the largest axis ($r_{\text{max}} = \max(a, c)$) of the ellipsoid. Additionally, we also consider the collision kernel at the edge of a sphere with the same volume as the ellipsoid ($r_{\text{mean}} = r = a^{\beta^{1/3}}$), i.e. a kind of ‘mean’ radius of the ellipsoids assuming random orientation.

In brief, the exact dynamic collision kernel $\Gamma^D$ for ellipsoids will be interpreted using the kinematic kernels $\Gamma^K$ at three relevant radii since $\Gamma^K$ provides additional information on the impact of turbulence, namely the RDF and the RRV.

3.3. Results

Initial evidence of the validity of the description in § 1 is given in figure 4. As an example, the trajectories and orientations of two identical ellipsoids before a collision
are visualized (figure 4a). Additionally, the cosine of the angle between the symmetry axes of the two ellipsoids is plotted as a measure for their alignment (figure 4b). As sketched in figure 1, the initially similarly oriented ellipsoids are rotated differently by a turbulent eddy such that the ellipsoid starting above can overtake the other ellipsoid due to its higher settling velocity.

Figure 5 shows the dynamic collision kernel $\Gamma^D$ (2.3) and the kinematic collision kernel $\Gamma^K$ (2.4) of ellipsoids with different aspect ratios $\beta$ but identical volumes. The $\Gamma^D$ and $\Gamma^K$ value for $\beta = 1$ is in accordance with earlier simulations of spherical particles (Kunnen et al. 2013). Compared with $\beta = 1$, $\Gamma^D$ is clearly larger for $\beta \neq 1$. Thus, the particle shape has an influence on the collision rate and the transition to higher collision rates is quite pronounced. There are no results in the literature for direct comparison. However, the impact of the particle shape on the collision rate is not entirely unexpected as the particle motion is known to depend on the shape (Siewert et al. 2014b). Parsa et al. (2012) concluded from their investigations on the rotation rates of neutrally buoyant ellipsoids that the model of thin rods or disks is generally more accurate for non-spherical particles than the assumption of equivalent spherical particles. The results of this study support this conclusion for the collision rates of inertial ellipsoids.

The kinematic collision kernel $\Gamma^K$ is depicted using $r_{\text{mean}}$ as collision radius in figure 5. Additionally, the values of $\Gamma^K$ obtained by $r_{\text{min}}$ and $r_{\text{max}}$ are shown as lower and upper bounds in an error-bar-like plot. These upper and lower bounds cover quite a large range since nominally $\Gamma^K \sim r^2$ (see (2.4)). However, the same trend of an increased collision kernel for non-spherical particles can be identified for $\Gamma^K$ and $\Gamma^D$. Note that $\Gamma^K$ at $r_{\text{mean}}$ matches the exact $\Gamma^D$ quite well, in particular for prolate ellipsoids ($\beta > 1$). In the following the two contributing factors RRV and RDF of $\Gamma^K$ are investigated.
Collision rates of small ellipsoids settling in turbulence

Figure 5. Collision kernels $\Gamma^D$ (filled symbols) and $\Gamma^K$ (open symbols) as a function of ellipsoid aspect ratio $\beta$ for ellipsoids settling in turbulence at $R_\lambda = 20.5$. The kinematic kernel $\Gamma^K$ is based on the collision radius $r_{\text{mean}}$; the error bars indicate the values of $\Gamma^K$ obtained for $r_{\text{min}}$ (lower limit) and $r_{\text{max}}$ (upper limit).

Within the dissipation range the dependence of the RRV and the RDF on the particle separation distance is known to follow a power-law behaviour for inertial and motile spheres (Bec et al. 2010; Saw et al. 2012; Durham et al. 2013). Hence, a similar spread is expected for the values obtained at the distances $2r_{\text{min}}$, $2r_{\text{mean}}$, and $2r_{\text{max}}$. However, as depicted in figure 6 the values for the three distances are quite close to each other allowing unambiguous statements since the lengths of the ellipsoidal semi-axes are of the same order of magnitude.

The RDF of ellipsoids ($\beta \neq 1$) is roughly a factor of two lower than for spheres ($\beta = 1$) (figure 6b). Apparently, the tendency to cluster is less strong, indicating the variation in response to changes in the flow field due to the importance of the orientation. Very recently, a similar reduction of clustering has been reported for motile prolate-shaped micro-organisms (Zhan et al. 2014). Although these organisms are not heavier than the fluid and do not settle due to gravity, they nevertheless cross the streamlines of the fluid by swimming. Hence, the dynamics of, especially, gyrotactical micro-organisms are found to share similarities with the dynamics of inertial particles (Durham et al. 2013).

However, in confirmation of the theoretical considerations from § 2.2 the RRV is much larger for non-spherical particles than for spheres, see figure 6(a). The qualitative comparison of these results with the theoretical distribution in figure 3 shows that the theoretical prediction yields the correct shape of the distribution. The increase in the RRV is much more pronounced than the decrease of the RDF such that $\Gamma^K$ of ellipsoids is up to 6.5 times larger than that of spherical particles. This increase of the collision rate can have a huge impact on the evolution of particle spectra as they occur, for example, in planetary-forming discs or mixed-phase and ice clouds, since collision-induced growth is typically a chain-process with exponential growth rates due to the dependence of collision probability on the particle size. The volume in which to collect other particles grows with the particle size, (2.4), and with the increased particle settling velocity, (2.5). For instance, it was shown that the time to the onset of precipitation reduces by 40% if the collision probability of the smallest drops is moderately enhanced by turbulence, e.g. by a factor of 2 (Xue et al. 2008).
Figure 6. Contributions to the kinematic kernel $\Gamma^K$ for the same case as in figure 5 as a function of the aspect ratio $\beta$: (a) mean radial relative velocity $\langle |w_r| \rangle$ (RRV); (b) radial distribution function $g_{11}$ (RDF).

To provide evidence that the higher RRV is due to different orientations at contact, we have computed the probability density function (PDF) of the cosine of the angle between the symmetry axes $c_1$ and $c_2$ of the two colliding ellipsoids, see the inset in figure 4(b). The spherical ellipsoids are assigned a virtual symmetry axis which is subsequently tracked. In figure 7(a–c) these PDFs are shown for oblate ellipsoids at $\beta = 0.25$, spherical particles ($\beta = 1$), and prolate ellipsoids ($\beta = 4$). Unlike spherical particles that have no preferred orientation at contact, both oblate and prolate ellipsoids display a preferred parallel alignment ($\cos(\alpha) = 1$) at contact. Since the particle time scales are small a parallel orientation at contact is expected given that the two ellipsoids experienced practically the same local flow field. However, there is a non-zero probability that ellipsoids have different orientations at contact. To visualize the impact of the contact angle on the RRV, we calculate the RRV conditionally averaged by the contact angle. These results are plotted in figure 7(d–f) for oblates, spheres, and prolates, respectively. Due to the high intermittency of the RRV (Bec et al. 2010) and the PDF of the contact angle, the conditional average shows a rather large scatter. Nevertheless, the results show a clear tendency. While the conditional RRV for spheres is constant at a low level, the conditional RRV of oblate and prolate ellipsoids reveals a strong dependence on the contact angle. It is much higher for non-aligned colliding ellipsoids for which $\cos(\alpha)$ is less than approximately 0.9. Hence, the collisions of non-aligned ellipsoids contribute a significant portion to the unconditioned mean value $\langle |w_r| \rangle$ although these collisions rarely occur.

To provide further evidence that the high collision rate is caused by the interaction of turbulence randomizing the particle orientation and gravity inducing orientation...
Collision rates of small ellipsoids settling in turbulence

FIGURE 7. (a–c) PDFs of the cosine of the collision angle $\alpha$ of the axes of symmetry $e_1$ and $e_2$ of two colliding ellipsoids. Three cases are considered: the simulations with gravity and turbulence are denoted turb + g, the simulations with turbulence and zero gravity are denoted turb; the theoretical case is denoted theo. Since the use of all three collision radii results in similar distributions, for clarity only the curve assuming $r_{\text{mean}}$ as collision radius is shown: (a) oblate ellipsoids ($\beta = 0.25$); (b) spheres ($\beta = 1$); (c) prolate ellipsoids ($\beta = 4$). (d–f) Values of the RRV $\langle |w_r| \rangle$ conditionally averaged by $\cos \alpha$ (solid lines as in a–c) and the corresponding mean values from figure 6(a) (dashed line): (d) oblate ellipsoids ($\beta = 0.25$); (e) spheres ($\beta = 1$); (f) prolate ellipsoids at $\beta = 4$.

dependence, we compare three cases: first, the theoretical case of randomly oriented ellipsoids settling in a quiescent fluid, the details of which are discussed in § 2.2; second, the previously discussed case of ellipsoids settling in turbulence; and third, an additional case of ellipsoids in turbulence but with gravity set to zero. For the
last case, the simulations described in § 3.1 are repeated for \( g = 0 \). The results are also summarized in figure 7. In figure 7(a–c) the PDFs of the collision angle are similar with and without gravity. As expected, without gravity collisions of unaligned ellipsoids are slightly less frequent since the uncorrelating influence of the differing settling velocities is absent. In the theoretical case the collision angle is random as prescribed.

While turbulence is responsible for the orientation distribution at contact, it is clear from figure 7(d–f) that without gravity the relative velocities of ellipsoids are as low as the relative velocities of spheres even for collisions of unaligned ellipsoids. In contrast, the theoretical prediction considering only gravitation-induced velocities matches the simulation with additional turbulence reasonably well. Reviewing the assumption made in the derivation of the theoretical RRV equation (2.7) in § 2.2, it can be stated that neglecting the turbulent fluctuation velocity differences compared to the gravitational settling velocity differences is indeed a good approximation for the conditional averaged RRV (figure 7d–f). However, the contact angle is not random, instead the nearby particles are mostly aligned (figure 7a–c). Hence, due to the collision angle PDFs the mean value of the theoretical RRV is too high and thus could not be compared quantitatively in figure 6. To accurately predict the RRV, the orientation distribution has to be understood and modelled. This complex problem should be addressed in future work. Nevertheless, since the clustering is neglected in the theoretical model and is thus underpredicted, the first-order model still is a better approximation of the shape-dependent ellipsoidal collision kernel than assuming a constant low kernel derived by equivalent spheres.

Similar to most theoretical and numerical studies on particles in turbulence (e.g. Squires & Eaton 1991; Wang & Maxey 1993; Sundaram & Collins 1997; Wang et al. 2000; Zhang et al. 2001; Falkovich et al. 2002; Bec et al. 2006; Wilkinson et al. 2006; Falkovich & Pumir 2007; Mortensen et al. 2008; Bec et al. 2010; Marchioli et al. 2010; Pumir & Wilkinson 2011; Parsa et al. 2012; Durham et al. 2013; Kunnen et al. 2013; Siewert et al. 2014b), we neglected the influence of the particles on the flow and the hydrodynamic interaction between nearby particles. Due to this simplification the computed geometric collision probabilities are only a qualitative representation of the real collision probabilities. However, the higher the relative velocity between two particles the less the time they have to adapt to the perturbations of the flow field induced by the approaching collision partner (Pinsky & Khain 1998). Consequently, the effect identified in this study is realistic and is expected to influence the evolution of particle size spectra.

4. Conclusion

To the best of our knowledge, we have, for the first time, investigated collisions of ellipsoidal particles settling in turbulence. It has been shown that the collision frequency of rotationally symmetric ellipsoids settling in turbulence is higher than that of spheres of the same volume. This originates from the combination of particle inertia, gravitational settling, and turbulence. Due to the orientation dependence of the settling velocity the particle velocity field can take multiple values, leading to an enhanced high collision rate compared to spheres.

It is reasonable that this effect applies to all types of non-spherical particles regardless of their actual shape since the prerequisite of orientation-dependent settling velocities is generally fulfilled. The principal open question is to what extent the particle shape affects the rotational inertia and with it the dynamic orientation distribution of the particles.
Acknowledgements

The funding of this project in the framework of the priority program SPP1276 METSTROEM by the German Research Foundation (DFG) under grant number SCHR 309/39 is gratefully acknowledged. The authors thank the High Performance Computing Center Stuttgart (HLRS) for the computing resources. We thank the anonymous reviewers for their remarks, which helped to improve the manuscript considerably.

REFERENCES


C. Siewert, R. P. J. Kunnen and W. Schröder


