Clustering and collision of inertial particles in random velocity fields

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The influence of clustering on the collision rate of inertial particles in a smooth random velocity field, mimicking the smaller scales of a turbulent flow, is analyzed. For small values of the ratio between the relaxation time of the particle velocity and the characteristic time of the field, the effect of clusters is to make more energetic collisions less likely. The result is independent of the flow dimensionality and is due only to the origin of collisions in the process of caustic formation.

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The transport of finite size particles in turbulent flows is a common occurrence in several environments: raindrops in clouds [1], plankton in oceans [2], sprays in industrial flows [3], to name some examples. Due to inertia, these particles undergo clustering phenomena that have been observed in numerical simulations [4], experiments [5], and have been the subject of substantial theoretical study [6,7,9–11].

Although contributing to particle segregation [12], spatial inhomogeneities in the turbulence do not appear to be an essential factor. What seems to be important is the ability of the particles to catch one another in their motion as they slip with respect to the fluid, a circumstance that is most evident in one dimension (1D) [13,14]. In more than 1D, the process is more complicated and an important role is played by the preferential concentration of heavy (light) particles in the strain (vortical) regions of the flow [6].

An important motivation for the interest in clustering is the contribution to particle collision and coalescence, and it has been suggested that this is an important ingredient in the process of rain formation [1,15]. What is observed is the simultaneous onset of concentration fluctuations and increased collision rates, when the relaxation time of the particle velocity relative to the fluid becomes of the order of the turnover time of the fastest turbulent eddies [15]. For sufficiently small (and sufficiently dense) spherical particles, this relaxation time is the Stokes time $\tau_S = 1/18 a^2 \lambda / \nu_0$, where *a* is the particle diameter, λ is the ratio of the particle to fluid density, and ν_0 is the kinematic viscosity of the fluid [16].

When inertia is sufficiently high, the so-called sling effect ensues [17]: particle and fluid trajectories detach on the scale of eddies with turnover time τ_s , and their velocity will determine the particle collision velocity.

The collision rate R_{coll} depends both on the particle concentration $n(\mathbf{x}, t)$ and on the relative velocity $\boldsymbol{\nu}$ in the particle pairs; for binary collisions

$$R_{\text{coll}} \sim a^2 \langle n(a)n(0) \rangle \langle \nu | r = a \rangle, \tag{1}$$

with **r** the particle separation. (Similar expressions will hold for the coalescence rate, with a more complicate function of $\boldsymbol{\nu}$ in the conditional average.) Thus, both the sling effect and clustering, through the factors $\langle \boldsymbol{\nu} | \mathbf{r} \rangle$ and $\langle n(a)n(0) \rangle$, respectively, may be expected to enhance collisions. It was suggested in [17,18], however, that the dominant contribution to collision may be the sling effect and there is even some indication [19] that clustering may hinder rather than enhance collisions.

The problem of how clustering and the dynamics of the two-particle velocity distribution in general influence each other, is far from trivial, with caustic formation potentially playing an important role [17,20]. The purpose of this Rapid Communication is to understand whether it is possible to identify a clustering contribution to the velocity dynamics, and if this is associated with collision enhancement or hindering.

Let us consider the dynamics of an inertial particle suspension in a smooth incompressible random velocity field $\mathbf{u}(\mathbf{x},t)$, with correlation time τ_E , variance $\langle u_{\alpha}^2 \rangle = \sigma_u^2$, $\alpha = 1, 2, 3$, and correlation length $r_v \sim \sigma_u \tau_E$. Particles in a turbulent flow, with τ_S shorter than the Kolmogorov time, here identified with τ_E , will see turbulence precisely in this way, and this is appropriate for most aerosols of atmospheric interest [1,17]. Conversely, the opposite regime $\tau_S > \tau_E$ could be interpreted as a model for the effect of eddies at scale r_v on particles with τ_S corresponding to the turnover time of larger eddies. This limit is more relevant for industrial flows than for rain formation, as the relative motion of larger droplets in clouds is dominated by the different gravitational settling velocities of droplets of different size [1].

The two regimes of large and small Stokes number S $= \tau_S / \tau_E$ are qualitatively different, with the clustering maximum occurring somewhere at $S \leq 1$ [6,21]. For small S, the particle phase is monodisperse in velocity over most of the fluid volume [7,8]. The sling effect, due to the spatial correlation of **u**, occurs in coherent way through the formation of caustics, i.e., regions of crossing of particle jets with different velocity [17]. The two-particle dynamics, relevant for the description of clustering and binary collision, is described by the equation for the velocity difference $\tau_S \dot{\boldsymbol{\nu}} + \boldsymbol{\nu} = \Delta_r \mathbf{u}$, $\Delta_{\mathbf{r}} \mathbf{u}(\mathbf{x},t) \equiv \mathbf{u}(\mathbf{x}+\mathbf{r},t) - \mathbf{u}(\mathbf{x},t), \text{ and, for } S \ll 1, \langle \nu^2 | r \rangle$ $\sim \langle |\Delta_{\mathbf{r}} \mathbf{u}|^2 \rangle \rightarrow 0$ for $r \rightarrow 0$ (clearly, $\langle \nu^2 | \infty \rangle = \sigma_{\nu}^2 = 2\sigma_{\nu}^2$). Neglecting caustics would lead to O(S) collision rates, as predicted in the theory of Saffman and Turner [22]. The multivalued velocity distribution in caustics appears to be crucial in producing high enough collision rates.

In the opposite limit $S \ge 1$, the particles are scattered by the velocity fluctuations they cross in their motion as if undergoing Brownian diffusion [23]. In the $S \ge 1$ limit, the velocity difference equation can be approximated by a stochastic differential equation (SDE) in the following form, choosing units such that $\tau_S = \sigma_u = 1$:

$$\dot{\nu}_{\alpha} + \nu_{\alpha} = b_{\alpha\beta}(\mathbf{r})\xi_{\beta}, \quad \dot{r}_{\alpha} = \nu_{\alpha}, \tag{2}$$

where $b_{\alpha\gamma}(\mathbf{r})b_{\gamma\beta}(\mathbf{r}) = (4/S)[g_{\alpha\beta}(0) - g_{\alpha\beta}(\mathbf{r})], g_{\alpha\beta}(\mathbf{r}) = \sigma_u^{-2}\langle u_{\alpha}(\mathbf{r},t)u_{\beta}(0,t)\rangle$, and ξ_{α} is the white noise, $\langle \xi_{\alpha}(t)\xi_{\beta}(0)\rangle = \delta_{\alpha\beta}\delta(t)$. In the incompressible case $\partial_{\alpha}g_{\alpha\beta}(\mathbf{r}) = 0$. For $S \ge 1$, the majority of particles pair at r=0, and will have been at $r \ge r_v$ for most of the previous time interval of length $\sim \tau_S$ of which they have memory, so it is possible to set, in the first approximation, $b(r) \simeq b(\infty)$. This leads to a Brownian collision dynamics with a velocity distribution of width $\sigma_v \sim S^{-1/2} \sigma_u$.

Let us consider the effect of clusters on the collision velocity of the particle pairs in the small Stokes number regime. This regime could be analyzed within an SDE approach, imposing an artificially short correlation time to the random field $\tau_E \ll \sigma_u/r_v$. This is a Kraichnan model regime [24], in which the role of effective correlation time is played by the diffusion time for a pair of tracers, $\tilde{\tau}_E = r_v^2/(\sigma_u^2 \tau_E)$, to reach separation r_v . We have therefore an effective Stokes number

$$\epsilon = \tau_S / \tilde{\tau}_E = \tau_S \tau_E \sigma_u^2 / r_v^2, \tag{3}$$

and it is possible to have a small- ϵ large-*S* regime, in which Eq. (2) continues to be valid. The small ϵ regime has been the subject of extensive study (see, e.g., [11,14,20]). For small ϵ , the particle phase is still monodisperse away from caustics, only with velocity not locally equal to that of the random field, as is instead (to first approximation) in the *S* $\ll 1$, $\tau_F \sim r_V / \sigma_u$ regime.

For small ϵ , Eq. (2) leads to **r** changing little in a time τ_s (the correlation time for $\boldsymbol{\nu}$) and caustics arise as extreme events, in which a strong fluctuation in the random field causes particle pairs to jump ballistically to zero separation in a time $\sim \tau_s$ [14,20]. Clusters affect the process privileging particle pairs that are initially closer, i.e., less energetic fluctuations in $\Delta_r \mathbf{u}$, leading to smaller collision velocities [25]. We give a quantitative description of this effect for D=1 and $|r| \ll r_v$.

For $\epsilon \rightarrow 0$, the shapes of the pair trajectories terminating with a given collision velocity will concentrate around the one that maximizes probability (no condition is imposed on the caustics in which the trajectories develop). To determine the most likely trajectory ending with collision velocity $\nu(t) = \overline{\nu}$ at t=0, one can proceed iteratively, from some initial guess for the separation history, say $r_0(t) = \overline{\nu}t$. (We assume immaterial particles, so that they can overlap without interaction.) For a smooth field, we can take for $|r| \leq r_v$, $(r) \approx 1$ $-\alpha(r/r_v)^2$ with $\alpha = O(1)$, which gives $b(r) \sim \epsilon^{1/2}r$. For $|r| \leq r_v$, at the *k*th step in the iteration procedure, the first of Eq. (2) will then read, apart from an O(1) factor in front of the right-hand side (RHS) $\dot{\nu}_k + \nu_k = \epsilon^{1/2} r_k \xi$, leading to the solution

$$\nu_k(t) = \epsilon^{1/2} \int_{-\infty}^t d\tau e^{\tau - t} r_k(\tau) \xi(\tau), \qquad (4)$$

where $\dot{r}_k = \nu_{k-1}$, $r_k(0) = 0$, k > 0. The minimum problem will be, therefore,

PHYSICAL REVIEW E 77, 065301(R) (2008)

$$\delta[\ln \mathcal{P}[\xi] + \lambda_k \nu_k(0)] = 0, \qquad (5)$$

where δ indicates variation in ξ , $\mathcal{P}[\xi]$ is the probability density function (PDF) of the history $\xi(t)$ with $t \in [-\infty, 0]$, λ_k is the Lagrange multiplier to enforce $\nu_k(0) = \overline{\nu}$, and the r_k entering ν_k is assigned from the previous iteration. From $\mathcal{P}[\xi]$ $=\exp(-\frac{1}{2}\int \xi^2(t)dt)$ and Eq. (4), the minimum problem, Eq. (5), leads to the history $\xi_k(t) = \lambda_k \epsilon^{1/2} e^t r_k(t)$.

Substituting ξ_k into Eq. (4) and imposing $\nu(0) = \overline{\nu}$ gives the velocity profile $\nu_k(t)$ in the function of r_k , which, substituting into $\dot{r}_{k+1} = \nu_k$ leads to the iterative relation for $r_k(t)$,

$$r_{k+1}(t) = \overline{\nu} \left\{ 1 - \left[\int_{-\infty}^{0} d\tau e^{2\tau} r_k(\tau) \right]^{-1} \times \left[\int_{-\infty}^{t} d\tau e^{2\tau - t} r_k^2(\tau) + \int_{t}^{0} d\tau e^{\tau} r_k^2(\tau) \right] \right\}.$$
 (6)

The iterative scheme can be implemented numerically and converges rapidly. In particular, the starting point of a jump terminating in a collision at velocity $\bar{\nu}$ is $r_{\bar{\nu}} \simeq \lim_{k\to\infty} r_k(-\infty)$ and one finds from Eq. (6) $r_{\bar{\nu}} \simeq -7\bar{\nu}\tau_s$. The rather large factor 7 implies that the jump does not start from a spatially localized "kick," rather, the sling acts over an $O(\bar{\nu}\tau_s)$ distance equivalent to that of the final free flight.

From the same condition $\nu(0) = \overline{\nu}$, one finds $\lambda_k = [\epsilon \int_{-\infty}^0 d\tau e^{2\tau} r_k(\tau)]^{-1} \overline{\nu}$, which, substituted into $\xi_k(t) = \lambda_k \epsilon^{1/2} e^t r_k(t)$, together with $r_k \sim \overline{\nu}$, gives for the noise history $\xi_k \sim \epsilon^{-1/2}$ and therefore the PDF of observing a collision velocity $\overline{\nu}$ in a given pair will be, for $a \ll r_{\overline{\nu}}$: $\rho_{\text{jump}}(\overline{\nu}|a) \simeq \rho_{\text{jump}}(\overline{\nu}|0) \sim \mathcal{P}[\xi_k] \sim \exp(-c/\epsilon)$, with *c* a constant that can be shown to be 1/6 in 1D [14]. The PDF of the collision velocity $\overline{\nu}$ in the given pair, generated by a jump originating at separation *r* will be instead $\rho_{\text{jump}}(\overline{\nu}|0) \delta(r - \overline{\nu}T)$, where $T \simeq 7\tau_s$.

Multiplying by the PDF $\rho(r)$ of finding a pair at separation *r*, and integrating over *r*, gives the PDF of a collision at velocity $\bar{\nu}$

$$\rho_{\rm coll}(\bar{\nu}) = \rho(r_{\bar{\nu}})\rho_{\rm jump},\tag{7}$$

with the cluster contribution contained in the PDF for the particle pair separation $\rho(r_{\bar{\nu}})$. A collision velocity $\bar{\nu}$ implies a permanence time $\propto |\bar{\nu}|^{-1}$ in an interval *dr*, and this allows one to write the collision velocity PDF (that is the collision rate at that velocity) in the form

$$\rho_{\text{coll}}(\overline{\nu}) \sim \rho(\overline{\nu}, a) |\overline{\nu}| = \rho(a) \rho(\overline{\nu}|a) |\overline{\nu}|.$$
(8)

This in turn can be substituted into Eq. (1) exploiting the relation, valid in *D* generic, $\langle n(\mathbf{r})n(0)\rangle = \Omega \bar{n}^2 \rho(\mathbf{r})$, with Ω the domain volume and \bar{n} the mean concentration.

In 1D, $\rho(r) \propto r^{-2}$ [14], so that $\rho_{\text{coll}}(\bar{\nu}) \propto \bar{\nu}^{-2}$, as confirmed in Fig. 1. In the absence of clustering, in comparison, the distribution would have been uniform and $\sim \exp(-c/\epsilon)$ up to $|\bar{\nu}| \sim r_v / \tau_s$.

This picture extends to D > 1, as the extremal trajectories are still straight lines, and the relevant parameter remains the separation $r_{\overline{\nu}}$ at the start of the jump. In this case the finite particle size must be taken into account and a jump ending in a collision will develop along a straight line that does not



FIG. 1. Collision velocity PDF for the 1D problem $\dot{\nu} + \nu = \epsilon^{1/2}(r+\alpha)\xi$, $\dot{r} = \nu$, compared to $\rho = \nu^{-2}$ (upper line). Values of the parameters $\epsilon = 0.04$ and $\alpha = 0.02$ (a finite molecular diffusivity is necessary to regularize the dynamics at $r \rightarrow 0$).

necessarily pass through the center of the other particle. The probability of a jump originating at **r** leading to collision will be proportional therefore to the angle with which a particle is seen at distance *r*, i.e., $(a/r)^{D-1}$. Nevertheless, if $a \ll r_{\bar{\nu}}$, the collision velocity PDF, i.e., the PDF for the velocity in the direction of the jump at the other particle position, could be approximated as $\rho_{\text{jump}}(\nu|a) \simeq \rho_{\text{jump}}(\nu|0)$.

Now, the number of particles in a shell at distance r will be $\propto \rho(\mathbf{r})r^{D-1}dr$, where the PDF $\rho(\mathbf{r})$, provided $\lim_{r\to 0} r^D \rho(\mathbf{r}) < \infty$, is related to the correlation dimension D_2 of the distribution by the equation $\rho(\mathbf{r})r^D \propto r^{-D}\langle N_r^2 \rangle \propto r^{D_2}$, with N_r the number of particles in a volume of linear size r. Taking the product of the different contributions, the probability of collisions at velocity between $\overline{\nu}$ and $\overline{\nu} + d\overline{\nu}$ therefore will be

$$\rho_{\text{coll}}(\bar{\nu})d\bar{\nu} \propto \rho_{\text{iump}}(\bar{\nu}|0)\rho(\mathbf{r}_{\bar{\nu}})a^{D-1}dr_{\bar{\nu}},\tag{9}$$

where $r_{\overline{\nu}} = \overline{\nu}T$ for some $T = O(\tau_s)$. If, as in the 1D case, $\rho_{\text{iump}}(\nu|0)$ is independent of ν , the following result will hold:

$$\rho_{\rm coll}(\bar{\nu}) \propto \bar{\nu}^{D_2 - D}.$$
 (10)

Simulating the trajectories of an ensemble of inertial particles in a 2D Kraichnan random field leads to the result in Fig. 2, which confirms the prediction of Eq. (10). The peak to the left is produced by the finite size of the particles, in the present case $a \approx 1/2056$ of the domain size. Its width is $\langle \nu^2 | a \rangle^{1/2} \sim a \sigma_{\nu} / r_{\nu}$ (the typical relative velocity at separation *a*) and its height is a factor $\sim \exp(c/\epsilon)$ above the scaling range to the right, which is associated with the jumps.

As illustrated in Fig. 3, the collisions actually take place between clusters. The scaling $D_2 < D$ causes closer clusters and therefore less energetic collisions to be more likely. Notice that, although clustering hinders high velocity collisions, higher velocities are actually more probable inside clusters. The reason is purely statistical: higher particle concentrations are produced where clusters collide, i.e., by definition a place where ν is larger.

For large Stokes numbers, collisions cease to occur as extreme events; hence, the correspondence between collision velocities and jump lengths disappears, and the predictions



PHYSICAL REVIEW E 77, 065301(R) (2008)

FIG. 2. Collision velocity PDF in 2D from a sample of 10^5 particles with ϵ =0.04, advected by a smooth Kraichnan random field in a square domain $3r_v \times 3r_v$. The almost straight line is $\rho(\mathbf{r}) = r^{-2} \langle N_r^2 \rangle$ (appropriately rescaled), corresponding to a correlation dimension $D_2 \simeq 1.45$.

of Eqs. (7) and (10) cease to be valid. In this limit, the particle velocity distribution ceases to be monodisperse pointwise (near caustics, it would be a superposition of discrete jets) and particle velocities at close separations are in the first approximation independent. It was suggested in [19] that concentration fluctuations are produced by slowly approaching particle pairs, which spend a significant time at separate out a cluster contribution in the velocity PDF $\rho(\boldsymbol{\nu}|\mathbf{r})$, analogous to the one identified in Eqs. (8)–(10), or equivalently in the relation $\rho(\bar{\boldsymbol{\nu}}, a) \propto |\bar{\boldsymbol{\nu}}|^{-1} \rho_{\text{jump}}(\bar{\boldsymbol{\nu}}|a)\rho(r_{\bar{\boldsymbol{\nu}}})$.

Notice that the simultaneous increase of $\rho(r)$ and decrease in $\langle \nu^2 | r \rangle$ as $r \to 0$ is not sufficient to conclude that concentration fluctuations are associated with smaller relative velocities; in fact, $\lim_{r\to 0} \langle \nu^2 | r \rangle = 0$ also for passive scalars in incompressible flows, in which case, concentration fluctua-



FIG. 3. A snapshot of the particle distribution from the numerical simulation of Fig. 2, superimposed to the pattern of relative velocities (the small segments), which identify the caustics. The length and direction of the segments correspond to the largest eigenvalue and associated eigenvector of the correlation matrix $\langle v_i v_j | \mathbf{x}, t \rangle$, calculated as average on the particles in a box of size *a* at **x**.

tions are absent. An alternative approach is therefore required.

As carried on in [26], a clustering part in $\rho(\overline{\nu},\overline{\mathbf{r}}) = \langle \delta[\nu(t) - \overline{\nu}] \delta[\mathbf{r}(t) - \overline{\mathbf{r}}] \rangle$ could be identified in the higher order contributions from the expansion of $\mathbf{r}(t)$ around the Brownian motion limit. The analysis in [26] indicates a strong dependence on compressibility of the random field, and that the conclusion of the present paper, that clustering decreases collision velocities, remains valid at large *S* only for compressible flows. As in the small ϵ regime, however,

this clustering contribution cannot be identified with the actual velocity distribution inside the clusters, and is more in the form of a nonlocal cluster contribution to the velocity dynamics.

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