RATE OF BREAKUP OF SMALL INERTIAL AGGREGATES IN HOMOGENEOUS TURBULENCE

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Abstract The hydrodynamic breakup of small inertial aggregates in homogenous and isotropic turbulence is studied through numerical simulations. Small inertial aggregates are subject to shear stress caused by the local velocity gradient and drag stress caused by the relative velocity of the aggregate and the fluid flow. In our simulations, we follow aggregates moving through the flow and record the total stress acting on them. Breakup is assumed to occur when the total stress overcomes a predefined threshold representing the aggregate strength. By determining how long it takes for an aggregate to reach a stress exceeding its strength for the first time, we are able to derive a breakup rate. It is found that with increasing aggregate inertia, the drag stress rapidly becomes the dominant stress resulting in an increase of the breakup rate with increasing the aggregate inertia.

Breakup of suspended aggregates is a ubiquitous phenomenon in particle systems and plays an important role in many industrial and environmental processes, e.g. in the aggregation of polymeric colloidal particles or in the flocculation operations in wastewater treatment, breakup limits aggregate growth and leads to a stationary aggregate size distribution. Likewise, in the transport of sediments in river estuaries, breakup of suspended flocks alters the size distribution and crucially influences flock settling. In other applications, conditions are designed to facilitate breakup such as in the dispersion of inhalation drugs. Breakup of suspended aggregates is driven by two mechanisms: In impact breakup, aggregate breakup is caused by energetic collisions with solid objects such as walls, moving equipments (e.g. impeller blades) or other particles. Impact breakup is the dominant mechanism for large and strong agglomerates such as found in powder processing or industrial crystallization. In hydrodynamic breakup, aggregate breakup is caused by viscous stress acting on the aggregate. Hydrodynamic breakup is the dominant mechanism for small and weak aggregates where the constituting particles are hold together by Van der Waals or electrostatic forces.

In this work the breakup of small inertial aggregates due to hydrodynamic stress in homogeneous and isotropic turbulence is investigated, where by small we mean that the Reynolds number, based on the characteristic particle velocity and particle size, is small with respect to unity. Hydrodynamic breakup in turbulence is a challenging problem as the viscous stress acting on the aggregate is subject of strong fluctuations, and conditions where the hydrodynamic stress overcomes the cohesive strength of the aggregate occur only intermittently and with timescales controlled by turbulent fluid and particle motions. The aim of our study is the determine the frequency at which the hydrodynamic stress acting on an aggregate moving in a turbulent flow overcomes a predefined threshold value representing the aggregate strength. The resulting frequency is referred to as aggregate breakup rate which in this work is determined as a function of the aggregate strength.

For small inertial aggregates, the hydrodynamic stress acting on the aggregate is comprised of two contributions, namely the shear stress caused by the local fluid velocity gradient at the position of the aggregate, and the drag stress caused by the velocity difference between the aggregate and the fluid flow. Expressions for these two stresses are readily obtained by considering the total stress exerted on a spherical surface encompassing the aggregate [3]. The resulting expression for the shear stress reads as:

$$\sigma_\varepsilon = \sqrt{\frac{2}{15}}\mu\left(\frac{\varepsilon}{\nu}\right)^{1/2}, \tag{1}$$

where ε is the local energy dissipation, ν is the kinematic viscosity, and μ is the dynamic viscosity. The drag stress is proportional to the Stokes drag divided by the particle surface area:

$$\sigma_{St} = \frac{2}{3}\mu\frac{|\boldsymbol{v}-\boldsymbol{u}|}{R}, \tag{2}$$

where $\boldsymbol{v}$ is the aggregate velocity, $\boldsymbol{u}$ is the fluid velocity, and R is the aggregate radius. The total stress acting on the aggregate is given by the combination of the two:

$$\sigma = \sigma_\varepsilon + \sigma_{St}. \tag{3}$$

From Eqs. (1) – (3) it is seen that the hydrodynamic stress acting on an aggregate depends on the way the aggregate moves through the flow and how it samples turbulence. The motion of a small aggregate in a turbulent flow depends on the aggregate size and its density difference with respect to the fluid. These quantities give raise to two characteristic numbers, i.e. a density ratio $\beta = 3\rho_f/(2\rho_p + \rho_f)$ where ρ_p and ρ_f are the aggregate and fluid density, respectively, and the Stokes number $St = \tau_p/\tau_\eta$, where $\tau_p = R^2/(3\beta\nu)$ is the kinematic time scale of the aggregate, R is the aggregate radius, and τ_η is the Kolmogorov time scale. In the present work we considered heavy aggregates with $\rho_p/\rho_f \in (8,\, 2000)$ and sizes $R/\eta \in (0.02,\, 0.34)$ where η is the Kolmogorov length scale, resulting in St varying in between 0.16 and 40 and

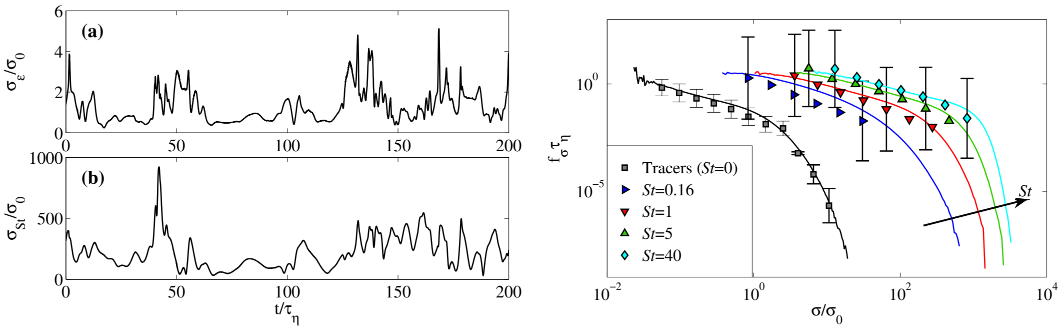

Figure 1. (Left) Time series of (a) shear stress and (b) drag stress along an aggregate trajectory, $St = 3$ and $R/\eta = 0.1$. (Right) Breakup rate as a function of the aggregate strength for an aggregate size of $R/\eta = 0.1$ and St ranging from 0 to 40. Symbols refer to exit time measurements while solid lines show a proxy [1]. In all panels, the hydrodynamic stress is normalized by σ_0, the average shear stress experienced by a tracer particle. τ_η is the Kolmogorov time scale.

β varying in between 10^{-4} and 10^{-2}. The small values of β allows for neglecting the added mass term in the equation of motion of a particle in turbulence. Aggregate trajectories are then obtained by evolving point-like inertial particles as done in a previous work [2]. In the simulations in [2] stationary and homogeneous isotropic turbulence with $R_\lambda \sim 400$ was realized in a periodic domain with 2048^3 grid points. Once the flow was stationary, point particles were injected and evolved over two eddy turnover times. In the context of the aggregates studied in this work, the simulation mimics a diluted suspension of inertial aggregates that are small with respect to the Kolmogorov size.

Fig. 1 (right) shows the shear stress and the drag stress along an aggregate trajectory for an aggregate of size $R/\eta = 0.1$ and $St = 3$. Both the shear stress and the drag stress are strongly fluctuating, with intense but short lived bursts occurring intermittently. Regions for intense shear stress coincide with regions of intense drag stress, however, the occurrence of peak stress varies among the two signals. Also, it is noticed that already for an aggregate with $St = 3$ the drag stress due to the velocity difference exceeds the shear stress by three orders of magnitude, making the drag the dominant mechanism for aggregate breakup. For measuring the aggregate breakup rate the scheme introduced in our previous work was applied [1]. In operative terms this reads as follows: (i) Consider a stationary homogenous flow. At a time t_0 a given number of aggregates is released at random into the flow. (ii) Aggregates released at a point where the local hydrodynamic stress exceeds the predefined threshold $\sigma_{\rm cr}$ representing the aggregate strength are ignored as breakup would have already occurred before the aggregates could have reached that point. (iii) Each of the remaining aggregates is followed in time until the local hydrodynamic stress exceeds the aggregate strength $\sigma_{\rm cr}$. The time lag from release until the breakup defines the exit-time $\tau_{\sigma_{\rm cr}}$ for that aggregate. (iv) Fragments formed upon breakup of an aggregate are discarded. The breakup rate for the given aggregate strength is then given by the inverse of the mean of the exit-time, given by the ensemble average over many time histories, i.e. $f_{\sigma_{\rm cr}} = 1/\langle\tau_{\sigma_{\rm cr}}\rangle$.

Fig. 1 (left) shows the breakup rate $f_{\sigma_{\rm cr}}$ as a function of the aggregate strength $\sigma_{\rm cr}$ for aggregates of size $R/\eta = 0.1$ and density varying from $\rho_p/\rho_f = 8$ to 2000. The Stokes number corresponding to these aggregates varies from $St = 0.16$ to 40. For a fixed Stokes, the breakup rate shows power law like behavior for a weak aggregate strength that terminates with a sharp super-exponential cut-off as the aggregate strength is increasing. With increasing Stokes, the velocity difference between the aggregate and the fluid flow increasing causing the drag stress to increase. This increase in the drag stress has twofold consequences for the breakup rate. On the one hand, for a fixed aggregate strength the breakup rate increases. On the other hand, the sharp cut-off at high aggregate strength moves to higher values. Results are compared to a quasi-Eulerian proxy [1] shown by the solid lines in Fig. 1 (left). For small and large St the quasi-Eulerian proxy is in good agreement with the exit time measurements, while for intermediate St there is some deviations.

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