EFFECTIVE DIFFUSION AND DISPERSION OF INERTIAL PARTICLES IN FLOWING FLUIDS

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Abstract We perform an analytical study of the inertial-particle dynamics in the limit of small but finite inertia, in incompressible flows, exploring two specific issues. First, by means of a multiscale expansion, we analyse the particle effective diffusivity, and in particular its dependence on Brownian diffusivity, gravity and particle-to-fluid density ratio. We identify some cases of anomalous diffusion. Secondly, we investigate the concentration of particles continuously emitted from a point source with a given exit velocity distribution. The anisotropy of the latter turns out to be a necessary factor for the presence of a correction (with respect to the corresponding tracer case) at order square root of the Stokes number. In both cases, we obtain forced advection–diffusion equations for auxiliary quantities in the physical space, thus simplifying the problem from the full phase space to a system which can easily be solved numerically.

THE DYNAMICS OF INERTIAL PARTICLES

Let us consider a single, small, spherical inertial particle, of mass density ρ_p and radius r, subject to Brownian diffusivity (κ) and gravity ($\boldsymbol{g}$), and carried by a fluid with density ρ_f and kinematic viscosity ν. Let us focus on an incompressible flow $\boldsymbol{u}(\boldsymbol{x},t)$ and let us define two usual quantities, the density coefficient $\beta \equiv 3\rho_\mathrm{f}/(\rho_\mathrm{f}+2\rho_\mathrm{p})$ and the Stokes time $\tau \equiv r^2/3\nu\beta$. The particle position $\boldsymbol{X}(t)$ and covelocity $\boldsymbol{V}(t) \equiv \dot{\boldsymbol{X}}(t) - \beta\boldsymbol{u}(\boldsymbol{X}(t),t)$ evolve according to [1, 2]:

$$\begin{cases} \dot{\boldsymbol{X}}(t) = \boldsymbol{V}(t) + \beta\boldsymbol{u}(\boldsymbol{X}(t),t) \\ \dot{\boldsymbol{V}}(t) = -\dfrac{\boldsymbol{V}(t)-(1-\beta)\boldsymbol{u}(\boldsymbol{X}(t),t)}{\tau} + (1-\beta)\boldsymbol{g} + \dfrac{\sqrt{2\kappa}}{\tau}\boldsymbol{\eta}(t)\ , \end{cases} \tag{1}$$

where $\boldsymbol{\eta}(t)$ is the standard white noise mimicking thermal fluctuations, the added-mass term has been accounted for in a simplified way, and the action of the fluid has been modelled via the Stokes viscous drag. The Basset, Faxén, Oseen and Saffman corrections have been neglected, as well as any interaction with boundaries or other particles and any more feedback on the fluid. The Fokker–Planck equation for the particle concentration $p(\boldsymbol{x},\boldsymbol{v},t)$ in the phase space reads:

$$\left\{\frac{\partial}{\partial t} + \frac{\partial}{\partial x_\mu}(v_\mu + \beta u_\mu) + \frac{\partial}{\partial v_\mu}\left[\frac{(1-\beta)u_\mu - v_\mu}{\tau} + (1-\beta)g_\mu\right] - \frac{\kappa}{\tau^2}\frac{\partial^2}{\partial v_\mu \partial v_\mu}\right\} p = F(\boldsymbol{x},\boldsymbol{v},t)\ , \tag{2}$$

with F denoting any possible particle source. When F is different from 0, the phase-space concentration p and its physical-space counterpart $P(\boldsymbol{x},t) \equiv \int \mathrm{d}\boldsymbol{v}\, p(\boldsymbol{x},\boldsymbol{v},t)$ are complicated functions which describe the particle dispersion following their emission [3]. In the absence of sources, $F=0$ and the behaviour of p is easier to describe, but is still nontrivial because it gives rise to interesting particle transport properties, such as their terminal settling velocity [4, 5] and effective diffusivity. Making use of the characteristic length and speed scales of the fluid flow, L and U respectively, it is customary to adimensionalize the problem and to express the results in terms of three adimensional numbers: $\mathrm{St} \equiv \tau U/L$ (Stokes), $\mathrm{Pe} \equiv LU/\kappa$ (Péclet) and $\mathrm{Fr} \equiv U/\sqrt{gL}$ (Froude).

RENORMALIZED (ANOMALOUS?) EDDY DIFFUSIVITY

Let us first assume $F=0$ in (2), in the presence of a zero-mean flow field, steady or periodic in time (with period T) and cellular in space (with cell size L) [6]. Investigating the particle dynamics at large length and time scales, $\gg L$ and $\gg T$ respectively, we can use the multiple-scale technique [7, 8] and isolate a possible ballistic degree of freedom related to the terminal velocity $\boldsymbol{w}$, in order to be left with a purely diffusive large-scale behaviour:

$$\frac{\partial}{\partial \mathcal{T}}\mathcal{P}(\boldsymbol{\mathcal{X}},\mathcal{T}) = K_{\mu\nu}\frac{\partial^2}{\partial \mathcal{X}^\mu \partial \mathcal{X}^\nu}\mathcal{P}(\boldsymbol{\mathcal{X}},\mathcal{T})\ . \tag{3}$$

Here, $\mathcal{P}$ represents the particle concentration in the newly-introduced slow variables $\boldsymbol{\mathcal{X}} \equiv \epsilon\boldsymbol{x}$ and $\mathcal{T} = \epsilon^2 t$ (ϵ being the well-known scale-separation parametre), while the effective-diffusivity tensor results from an integration on the original fast variables (viz. on the cell periodicity in space and time) [9]:

$$K_{\mu\nu} = \int_0^T \frac{\mathrm{d}t}{T}\int \mathrm{d}\boldsymbol{x}\int \mathrm{d}\boldsymbol{v}\ [v_\mu + \beta u_\mu(\boldsymbol{x},t) - w_\mu]\, q_\nu(\boldsymbol{x},\boldsymbol{v},t)\ . \tag{4}$$

The vector $\boldsymbol{q}(\boldsymbol{x},\boldsymbol{v},t)$ satisfies the so-called cell problem, i.e. an auxiliary equation with the same operatorial structure of (2) (replacing p with $\boldsymbol{q}$) but with a right-hand side given by $[\boldsymbol{v}+\beta\boldsymbol{u}(\boldsymbol{x},t)-\boldsymbol{w}]\,p(\boldsymbol{x},\boldsymbol{v},t)$. The resolution of the full problem (which cannot be achieved analytically, except for some very simple flows) is prohibitive also numerically, because it involves $2d+1$ variables, d being the usual space dimension. However, in the limit of small inertia, the covelocity degree of freedom decouples from space and time, and we are left with a St-expansion of the particle diffusivity:

$$K_{\mu\nu} = \mathrm{Pe}^{-1}\delta_{\mu\nu} + \int_0^T \frac{\mathrm{d}t}{T}\int \mathrm{d}\boldsymbol{x}\ [u_\mu Q_\nu + \mathrm{St}(1-\beta)u_\mu u_\nu] + \mathrm{O}(\mathrm{St}^2)\ , \tag{5}$$

where the vector $\boldsymbol{Q}$ itself results from an expansion $\boldsymbol{Q}(\boldsymbol{x},t) = \boldsymbol{Q}_0(\boldsymbol{x},t) + \mathrm{St}\boldsymbol{Q}_1(\boldsymbol{x},t) + O(\mathrm{St}^2)$ (notice that, in this case, only integer orders appear). Every coefficient of the latter expansion obeys forced advection–diffusion equations — obtained from solvability conditions — which can be solved analytically e.g. for the Kolmogorov parallel shear flow, or numerically for more general cases (this is a relatively easy task, involving only $d+1$ variables). The equation for $\boldsymbol{Q}_0$ is

$$\left(\frac{\partial}{\partial t} + u_\mu\frac{\partial}{\partial x_\mu} - \mathrm{Pe}^{-1}\frac{\partial^2}{\partial x_\mu \partial x_\mu}\right)\boldsymbol{Q}_0 = \boldsymbol{u}(\boldsymbol{x},t)\ , \tag{6}$$

thus making the $O(\mathrm{St}^0)$ in $K_{\mu\nu}$ coincide with the well-known tracer limit [10]. We also found the equation for $\boldsymbol{Q}_1$, but we do not report it here due to its length. We just mention that gravity may pop out at $O(\mathrm{St})$ for finite Fr, or even down at the (tracer-like) order St^0 for finite $\boldsymbol{w}$. Moreover, for random flows, we are able to identify some situations of anomalous diffusion, in specific ranges of the spatial and temporal exponents of the fluid velocity spectrum (in Fourier space).

DISPERSION FROM A POINT SOURCE

Now, let us consider a continuous emission at a constant rate T^{-1} from a localized particle source, which for the sake of simplicity can be considered as punctual and located in the origin. A typical example is provided by a chimney emitting some particulate in the atmosphere, even if in this case κ should be replaced with some eddy diffusivity in order for our model to work; other instances where κ is really the Brownian value are given by the emission of microparticles in a channel (e.g. from a syringe) and the deposition of powders in filters or in the lung alveoli. Denoting with $f(\boldsymbol{v})$ the emission distribution in terms of the particle covelocity, we have $F = T^{-1}\delta(\boldsymbol{x})f(\boldsymbol{v})$. Again, the resolution is possible upon performing a power-series expansion (here, of the concentration and with half-integer orders) at small inertia, giving:

$$P(\boldsymbol{x},t) = P_0(\boldsymbol{x},t) + \mathrm{St}^{1/2}P_1(\boldsymbol{x},t) + O(\mathrm{St})\ , \tag{7}$$

where P_0 and P_1 satisfy equations like (6), but where the right-hand sides are

$$R_0 \equiv \frac{L}{TU}\delta(\boldsymbol{x}) \quad \text{and} \quad R_1 \equiv \frac{L}{TU}\mathrm{Pe}^{-1/2}\frac{\partial\delta(\boldsymbol{x})}{\partial x_d}\int \mathrm{d}\mathcal{V}\,\mathcal{V}^d \mathrm{e}^{-\mathcal{V}^2/2}\mathcal{Q}(\mathcal{V})\ ,$$

respectively. The equation for P_0 with R_0 corresponds to the well-known tracer limit for zero inertia. In the presence of inertia, the leading correction is generally speaking at $O(\mathrm{St}^{1/2})$, and is given by P_1 with the above expression for R_1, in which $\mathcal{Q}(\mathcal{V})$ obeys a quantum-harmonic-oscillator-like equation. The latter is forced by $f(\boldsymbol{v})$ — more precisely, by the first anisotropic sector in its decomposition onto spherical harmonics — and for a Gaussian covelocity distribution can explicitly be solved, in which case x_d represents the axis along the mean value of the emission (e.g. it points upwards for the case of pollutants released from a smokestack). The density coefficient only appears in the full expression $p(\boldsymbol{x},\boldsymbol{v},t)$ and thus in the derivation of the particle transport properties; on the contrary, gravity has no explicit role at this stage, unless one considers the simultaneous limits $\mathrm{St}\to 0 \leftarrow \mathrm{Fr}$, combined to result in a finite terminal velocity in order to take sedimentation into account. However, it is crucial to point out that, if the covelocity emission is isotropic ($f(\boldsymbol{v}) \mapsto f(v)$), both $\mathcal{Q}$ and P_1 vanish, and from (7) the leading correction becomes $O(St)$.

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