

Transport, mixing and agglomeration of particles in turbulent flows

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Abstract. This paper describes methods and approaches that have been used to simulate and model the transport, mixing and agglomeration of small particles in a flowing turbulent gas. The transported particles because of their inertia are assumed not to follow the motion of the large scales of the turbulence and or the motion of the small dissipating scales of the turbulence. We show how both these behaviours can be represented by a PDF approach analogous to that used in Classical Kinetic Theory. For large scale dispersion the focus is on transport in simple generic flows like statistically stationary homogeneous and isotropic turbulence and simple shear flows. Special consideration is given to the transport and deposition of particles in turbulent boundary layers. For small scale transport the focus is on how the the small scales of turbulence together with the particle inertial response enhances collision processes like particle agglomeration. In this case the importance of segregation and the formation of caustics, singularities and random uncorrelated motion is highlighted and discussed.

Keywords: inertial particles, turbulence, pdf approach, segregation, dispersion

1. Introduction

This paper is about ways of simulating and modelling the transport of small particles in a turbulent flow. More particularly it's about modelling and simulating the way the turbulence mixes and disperses these particles, the way it deposits and resuspends them from surfaces exposed to the flow and how it brings them closer together and enhances their collision processes as in particle agglomeration. Of particular concern will be the way these small particles respond to both the large and small scales of turbulence and how in turn this *inertial* response influences these various transport processes. This response is characterized by the particle Stokes number St which measures the particle response time to the typical time scale of the motion of the large or the small scales of the turbulence. We focus our attention on the motion of solid particles in a turbulent gas because the forces on the particles are simply expressed in terms of quasi-steady lift or drag dependent on the relative velocity between particle and local carrier flow. In the simple cases we wish to consider, the forces acting on the particles will simply be that derived from Stokes drag. Such particle suspensions are referred to here and elsewhere [45] as *turbulent aerosols* so that the mass loading of the aerosol particles is sufficiently low to ignore any way two-way coupling between the continuous gas¹ and particle dispersed phases.

¹ We will refer to this as the *carrier flow* or sometimes as simply the *fluid*



Turbulent aerosols are a feature of many industrial and environmental processes: from cloud droplets, mists and fogs to mixing and combustion processes in coal fire burners, and the release and dispersal of radioactive particles in a nuclear severe accident. They influence the weather and are key factors in controlling climate; they impact upon our health and longevity. So understanding how they behave, how they can be controlled is an important area of study. In all these processes the turbulence, both the large and small scales play a crucial role in determining their behaviour. How for instance the aerosol droplets or particles are formed by nucleation, grow or evaporate, how they mix and chemically react, and the way particles interact with surfaces exposed to the flow. Such processes are controlled by either the large scales or the small scales and in some cases by both scales acting together. An area of much investigation is the mechanism for warm-rain initiation and in particular the way droplet interaction with the small scales of turbulence in clouds leads to a droplet size distribution, much broader than one would expect from a closed adiabatic parcel model of droplet formation and growth. It is the small scales of the turbulence for instance that are responsible for the segregation or un-mixing of a turbulent aerosol where not only the scale is important but also the structure of the turbulence and the mixture of straining and vorticity within those scales.

In this short review of *particles in turbulence* we consider first those processes that are controlled by the large scales of the turbulence (typical of the size of the flow containment). The large scale motion influences and controls what is commonly referred to as one-particle dispersion and in this process the influence of the local mean shear for which the influence of the local mean shear is inextricably linked to the turbulence. It is what we mean by the transport of particles in complex flows where particles are transported both by the mean shear and the turbulence produced by the shear, both being spatially non uniform. However a consideration of the transport of particles in simple generic flows like statistically stationary homogeneous and isotropic turbulence and simple shear flows provide important insights into the way particles are transported in turbulent shear flows in general. A crucial consideration is the transport of particles in a turbulent boundary layer since the turbulence has an important rate limiting influence in transporting particles to a surface and special consideration will be given to this in this review.

The influence of the small scales of turbulence is referred to as two-particle dispersion since they influence the relative motion between two particles. It is at the small scales where the phenomenon of demixing of particle suspensions occur. This process has been the subject of intensive research over the last ten years. Partly because the small scales have a more universal structure far removed from the influence and complexity of local shear and partly because they are more amenable to analysis and to the construction of simple models. Simulation and analysis have revealed some important features such as the formation of caustics and the occurrence of singularities in the particle concentration field and the presence of random uncorrelated motion (RUM).

An important driving force in all these studies has been the need to provide a basic framework to handle the statistical nature of these processes and to use this to provide a two-fluid model of a particle-fluid mixture which treats the particle phase as a continuum and to develop a set of mass, momentum and energy equations for the dispersed phase analogous to those of the carrier phase. This is an essential element of turbulence modelling and an important element of the development and application of CFD. Over the last 20 years this has been the goal of the PDF approach, an approach analogous to statistical mechanics in that the quest is for a Master Equation analogous to the Maxwell-Boltzmann equation representing in this case the transport of particles in phase space - more particularly an equation that is appropriate for both one particle and two-particle transport. We begin our review of this subject by recalling the basic features of this approach, primarily because it is an approach that can in principle embody and provide models for the various processes as well in its own right provide insights into some of

the long term nature of these process that in some cases are difficult to resolve in simulation and in experiment.

2. PDF development

The probability density function (PDF) approach is a rational approach to modelling dispersed particle flows in the same way that classical kinetic theory is a rational approach for modelling gas flows. That is, there exists in both cases an underlying equation (a Master Equation) which, in a strictly formal way, can be used to derive both the continuum equations and constitutive relations of a gas or a dispersed phase of particles. In kinetic theory, the master equation is the well-known Maxwell–Boltzmann equation, whilst in the modelling of dispersed particle flows, it is known as the kinetic equation. There are currently two forms of the kinetic equation. In the first form, the pdf, as in Kinetic Theory, refers to the probability density that a particle has a certain velocity and position at a given time. This approach is referred to as the kinetic model (KM) approach. It was originally developed by Buyevich [4, 5, 6] and further developed since by a number of workers, most notably Reeks [34, 27, 28, 29], Hyland [20, 21], Swailes [41] Derevich [11], Zaichik [46] and Pozorski & Minier (1998) [26].

In contrast the second form of the PDF equation, first proposed by Simonin, Deutsch and Minier [36], refers to a more general PDF which includes the velocity of the carrier flow local to the particle as a phase space variable as well as the particle position and velocity. It is a development of the PDF approach used by Pope [17] based on a generalised Langevin model (GLM) for the equation of motion of the carrier flow encountered by a particle. It is referred to here as the GLM approach.

2.1. PDF equation for inert particles

To illustrate the differences and similarities between the KM and GLM approaches, let us consider the simplest case of the transport of inert non-reacting solid particles in a turbulent gas flow. To simplify the situation still further the drag acting on the particle is linearized with respect to the relative velocity, i.e.

$$\mathbf{F}_A \cong \underline{\bar{\eta}} \cdot (\mathbf{u} - \mathbf{v}) \quad (1)$$

where \mathbf{v} is the velocity of an individual particle at position \mathbf{x} at time t where the local flow velocity is $\mathbf{u}(\mathbf{x}, t)$ and $\underline{\bar{\eta}}$ is the tensor of net friction coefficients and given by

$$\underline{\bar{\eta}} = \frac{1}{2} \rho_g A C_D (\overline{Re_p}) |\bar{\mathbf{u}} - \bar{\mathbf{v}}| \quad (2)$$

where $\bar{\mathbf{v}}(\mathbf{x}, t)$ is the net particle mean velocity and $\overline{Re_p}$ is the value of the particle Reynolds number based on the net relative velocity between particle and local carrier flow. The equations of motion for the particle are

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \quad (3)$$

$$\frac{d\mathbf{v}}{dt} = \underline{\beta} \cdot (\mathbf{u} - \mathbf{v}) \quad (4)$$

where $\underline{\beta}$ is the inverse particle response tensor and given by $m^{-1}\underline{\bar{\eta}}$ for a particle of mass m . In the case of Stokes drag, the elements of $\underline{\beta}$ are constants of the motion and β_{ij}^{-1} are the corresponding particle response times to changes in flow. In addition to the particle equations of motion, the equation of motion of the carrier flow velocity \mathbf{u} along a particle trajectory is included, namely

$$\frac{du_i}{dt} = F_i(\mathbf{v}, \mathbf{u}, \mathbf{x}, t) \quad (5)$$

In the KM approach, one considers the continuum equations derived from an equation for the phase space probability density $\langle W \rangle(\mathbf{v}, \mathbf{x}, t)$ in which $\mathbf{u}(\mathbf{x}, t)$ is a random function of \mathbf{x}, t and \mathbf{v} and \mathbf{x} are independent random variables. In the GLM approach, the continuum equations are derived from a conservation equation for the phase space density $\langle P \rangle(\mathbf{v}, \mathbf{u}, \mathbf{x}, t)$ where $\mathbf{v}, \mathbf{u}, \mathbf{x}$ form a set of independent variables. The ensemble average $\langle \cdot \rangle$ means an ensemble of the instantaneous phase space densities W and P over all realizations of the flow velocity field. It is convenient to resolve $u_i(\mathbf{x}, t)$ and $F_i(\mathbf{v}, \mathbf{u}, \mathbf{x}, t)$ into mean and fluctuating parts,

$$u_i = \langle u_i \rangle + u'_i \quad F_i = \langle F_i \rangle + F'_i \quad (6)$$

so that the mean component is responsible for convection in phase space and the fluctuating part (due to the turbulence) is responsible for dispersion. Then the transport equations for mean values of W and P , namely $\langle W \rangle$ and $\langle P \rangle$, are

$$\frac{\partial}{\partial t} + \frac{\partial}{\partial x_i} v_i + \frac{\partial}{\partial v_i} \beta_{ij} (\langle u_j \rangle - v_j) \langle W \rangle = - \frac{\partial}{\partial v_i} \beta_{ij} \langle u'_j W \rangle \quad (7)$$

$$\frac{\partial}{\partial t} + \frac{\partial}{\partial x_i} v_i + \frac{\partial}{\partial v_i} \beta_{ij} (u_j - v_j) + \frac{\partial}{\partial u_i} \langle F_i \rangle \langle P \rangle = - \frac{\partial}{\partial u_i} \langle F'_i P \rangle \quad (8)$$

To solve these equations closure relations for $\langle u'_i W \rangle$ and $\langle F'_i P \rangle$ are required. We now consider the various forms that have been derived for these terms assuming that $\beta_{ij} = \beta \delta_{ij}$.

2.1.1. Closure approximation for a non-reactive gas-particle flows Kinetic model

Based on either the LHDI approximation (Reeks [29]) or the Furutsu Novikov formula (Swales & Darbyshire [41]), the closure approximation for the net flux $\langle u'_i W \rangle$ for particles with velocity \mathbf{v} and position \mathbf{x} at time t , is given by

$$\langle u'_i W \rangle = - \left(\frac{\partial}{\partial v_j} \mu_{ji} + \frac{\partial}{\partial x_j} \lambda_{ji} \right) \langle W \rangle + \kappa_i \langle W \rangle \quad (9)$$

where explicitly $\mu_{ij}(\mathbf{v}, \mathbf{x}, t)$ and $\lambda_{ij}(\mathbf{v}, \mathbf{x}, t)$ phase space diffusion coefficients that refer to diffusion in velocity and configuration space respectively and κ_i represents the components of a convective (body) force that depends on inhomogeneities in flow field (i.e it is zero for homogeneous turbulence). Both μ_{ij} , λ_{ij} and κ_i depends on the flow velocity correlation measured along particle trajectories that arrive at \mathbf{v}, \mathbf{x} at time t (See [29, 41]). Their values depend upon the local mean shearing of the flow.

Generalized Langevin Model GLM

Simonin, Deutsch and Minier (SDM) [36] derive an equation of motion for the fluid velocity along a particle trajectory by starting from the Langevin equation which Pope [17] has used as the analogue of the Navier Stokes equation for fluid point motion. Thus along a fluid point trajectory

$$\frac{du_i}{dt} = \alpha_{ij}(\mathbf{x}) (\langle u_j \rangle - u_j) + f_i(\mathbf{x}) + f'_i(t) \quad (10)$$

where $f_i(\mathbf{x})$ is the net viscous and pressure force per unit mass of fluid and $f'_i(t)$ is a white noise function of time. Both SDM and Pope consider the equation of motion in differential form because the white noise is assumed non differentiable. For convenience, it is assumed that the

white noise, like all turbulence related functions is differentiable. The equation of motion has white noise properties simply because it has a time scale much shorter than the time scale over which $\mathbf{u}(t)$ varies along a fluid point trajectory $O(\alpha^{-1})$. For future reference it is noted that

$$f_i(\mathbf{x}) = \frac{D_f \langle u_i \rangle}{Dt} + \frac{\partial \langle u'_j u'_i \rangle}{\partial x_j} \quad (11)$$

where

$$\frac{D_f}{Dt} = \frac{\partial}{\partial t} + \langle u_j \rangle \frac{\partial}{\partial x_j} \quad (12)$$

SDM use this relationship to generate an equation of motion for the fluid velocity along a particle trajectory. So if $\frac{d_p}{dt}$ is the time derivative of the fluid velocity along a particle trajectory and similarly if $\frac{d_f}{dt}$ is along a fluid point trajectory, then

$$\begin{aligned} \frac{d_p u_i}{dt} &= \left(\frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j} \right) u_i(\mathbf{x}, t) \\ &= \end{aligned} \quad (13)$$

SDM consider only the contribution from the gradient of the mean fluid velocity in this equation of motion for the fluid velocity along a particle trajectory. That is, they consider the equation

$$\frac{d_p u_i}{dt} = (v_j - u_j) \frac{\partial \langle u_i(\mathbf{x}, t) \rangle}{\partial x_j} + \alpha_{ij} (\langle u_j \rangle - u_j) + f_i(\mathbf{x}) + f'_i(t) \quad (14)$$

In effect this is equivalent to assuming that the contribution of the fluctuating fluid velocity gradient is absorbed into the white noise function $f'_i(t)$. Using the white noise function, the equation for $\langle P \rangle$ can be closed exactly; namely²

$$\begin{aligned} \langle F'_i(\mathbf{x}, t) P(\mathbf{v}, \mathbf{x}, \mathbf{u}, t) \rangle &= \langle f'_i(t) P(\mathbf{v}, \mathbf{u}, \mathbf{x}, t) \rangle \\ &= - \int_0^\infty \langle f'_i(0) f'_j(s) \rangle ds \frac{\partial \langle P \rangle}{\partial u_j} \end{aligned} \quad (15)$$

Then from Eq. (14), the equation for $\langle P \rangle$ used by SDM is:

$$\begin{aligned} &\frac{\partial \langle P \rangle}{\partial t} + \frac{\partial}{\partial x_i} v_i \langle P \rangle + \frac{\partial}{\partial v_i} \beta_{ij} (u_j - v_j) \langle P \rangle \\ &+ \frac{\partial}{\partial u_i} \left[\alpha_{ij} (\langle u_j \rangle - u_j) + f_i(\mathbf{x}) + (v_j - u_j) \frac{\partial \langle u_i \rangle}{\partial x_j} \right] \langle P \rangle \\ &= \int_0^\infty \langle f'_i(0) f'_j(s) \rangle ds \frac{\partial^2 \langle P \rangle}{\partial u_i \partial u_j} \end{aligned} \quad (16)$$

3. Dispersion in simple generic flows

The PDF equation can be used to obtain the continuum equations for the dispersed particle phase treated as a fluid. In the case of the GLM model an extra equation is provided for the mean carrier flow and covariance of the flow velocity seen by the particles which adds an extra layer of complication. Both approaches are equivalent to one another when the statistics of the fluid motion *seen* by the particle are Gaussian. We refer elsewhere to the explicit form for the continuum equation [32]. What is interesting is to say something about the form of the equation in simple generic flows because it gives some insights into the way particle are transported in more complex non-uniform shear flows. In particular there have been numerous experimental measurements and simulation on these basic particle-flows and it is useful to compare PDF predictions with these results.

² Note the closure is also exact if $\mathbf{f}''(t)$ is Gaussian non-white but will include gradients of $\langle P \rangle$ in \mathbf{x} and \mathbf{v} as well.

3.1. Dispersion in homogeneous isotropic turbulence

Much of the early work on particle dispersion in turbulent flows was directed towards evaluating or measuring the particle diffusion coefficient in statistical stationary homogeneous isotropic turbulence or grid generated decaying turbulence which could be considered as quasi-homogeneous and isotropic. We refer specifically to the seminal experimental measurements of Wells and Stock [44] who measured the particle dispersion in a turbulence flow field in which the particles were subjected to a mean drift due to an electric field. The experiment replicated the features that one would expect if particles were falling under gravity. The beauty of the experiment was that the settling velocity could be varied for any given particle size and in fact could be reduced to zero by applying an electric force in the opposite direction to gravity. In so doing they were able to separate out settling effects from inertial effects on the particle diffusion coefficient which is something that could not be done with gravitational settling alone (inertial and settling would always be inextricably linked). The important result from the PDF approach indicates that the diffusion is bound up with the form of the momentum equation in the same way as for Brownian motion (one recalls the way Einstein was able to deduce the Brownian diffusion coefficient using a similar approach [13]). Suppose you consider a system approaching equilibrium (but not at equilibrium). In that case we might legitimately ignore the inertial acceleration term in the momentum equation so that we have a particle flux described as a gradient diffusion equation. Because the underlying flow is homogeneous and terms that involved gradients of the flow itself can be ignored. The diffusion coefficient is given in the long term $t \rightarrow \infty$ by the expression

$$\epsilon = \tau_p \langle v^2 \rangle + \lambda \quad (17)$$

where $\tau_p = \beta^{-1}$ is the particle response time for Stokes drag and both particle mean square velocity $\langle v^2 \rangle$ and diffusion coefficient (obtained from the carrier flow velocity measured along a particle trajectory) are the long term equilibrium values. When the expression for λ and $\langle v^2 \rangle$ are substituted in this equation which both involve $\langle u'(0)u'(t) \rangle$ the carrier flow velocity auto correlation along a particle trajectory, you end up with the following remarkable result, namely

$$\epsilon = \int_0^\infty \langle u'(0)u'(t) \rangle dt \quad (18)$$

That is the diffusion coefficient does not depend explicitly upon its inertia, whatever the particle inertia, the form of the diffusion coefficient is the same. What difference there is depends on whether the carrier flow timescales along a particle trajectory are bigger or smaller than those along a fluid element trajectory. In fact particles with more inertia appear to have a diffusion coefficient that is greater than that for a fluid element or passive tracer. This is shown in Figure 1 based on the results obtained by Squires & Eaton [39] for particle diffusion in DNS isotropic homogeneous turbulence. The vertical axis is the ratio of the particle diffusion coefficient compared to that of the fluid or passive scalar. The calculations were done for a range of particle Stokes numbers St from 0.06 to 0.35 where Stokes number is the ratio of the particle response time τ_p to integral timescale of the flow T_f . You can see that for all the Stokes numbers the long time values of the diffusion coefficient are greater than that of the carrier flow, the greatest value being for $St = .33$ but with little difference between this value and the value for $St = 1.09$. The formula in Eq.(18) is also appropriate for particles settling under gravity or in an electric field as with the measurements of Wells and Stock [44]. The timescales of fluid motion along a particle trajectory depends upon the time it takes for a particle to move from one eddy to another in the flow field. The faster the particle moves the shorter the timescale of the fluid motion it encounters, assuming that the eddy lifetime is much longer than the transit time of the particle. If v_g is the settling velocity and l_e the spatial length scale then $l_e/v_g \ll \tau_e$

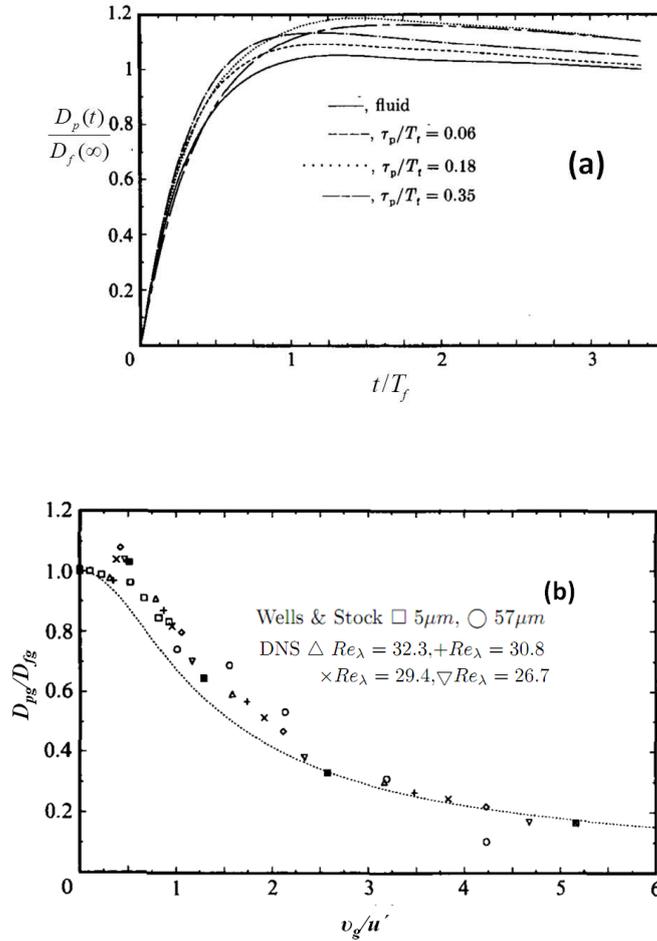


Figure 1. Ratio of particle diffusion coefficient to long term fluid element diffusion coefficient in homogeneous isotropic turbulence: DNS and experimental measurements, the influence of inertia τ_p/T_f and settling v_g/u' . Both plots are from Squires & Eaton[39]

where τ_e is the eddy decay time. Since $\tau_e \sim l_e/u'$ this implies $u'/v_g \ll 1$ in which case

$$\epsilon = \int_0^\infty R_E(0, v_g t) dt \quad (19)$$

where $R_E(t, x)$ is the carrier flow spatial velocity correlation (in a frame moving with the settling velocity \mathbf{v}_g with a separation x measured in the direction of gravity). ϵ in this case refers to the diffusion coefficient for diffusion in the direction of gravity.

This behaviour is reflected in Figure 1(b) where the long-time particle diffusion coefficient in the direction of gravity is shown as a function of the ratio v_g/u' again taken from Squires & Eatons' DNS calculations [39] and the measurements of Wells and Stock [44]. One further prediction of the PDF approach borne out by experiments and simulation is that the diffusion flux j_D is given by a Boussinesq approximation in the long term by

$$\mathbf{j}_D = \langle \rho \mathbf{v} \rangle = -\epsilon \cdot \frac{\partial \langle \rho \rangle}{\partial \mathbf{x}} \quad (20)$$

where $\langle \rho \rangle$ is average concentration at x the distance measured along any spatial direction, a result that reflects a Gaussian profile for the mean concentration for an instantaneous point source of particles.

Dispersion in a simple shear

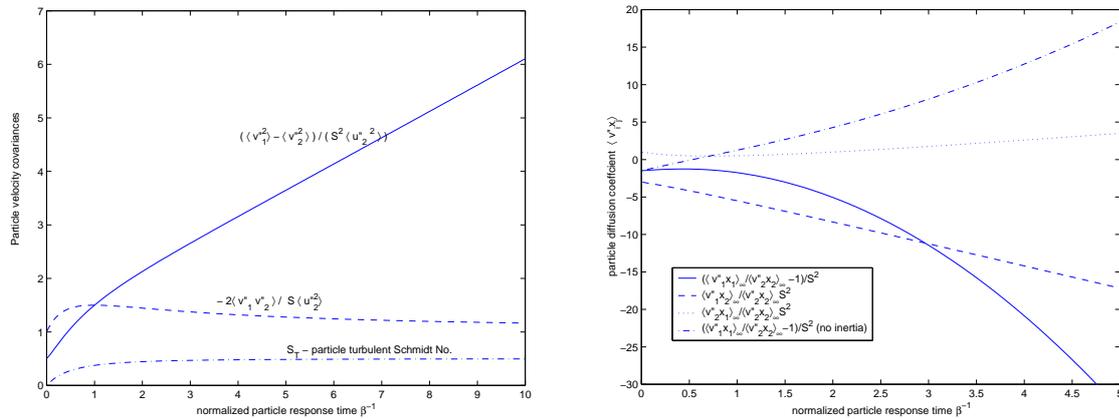
An important generic flow is particles transported in a simple shear flow. In single phase flow it is used to define what we mean by viscosity and the relation between shear stress and rate of straining of the flow. Using a simple model for the Reynolds shear stresses based on Pope's GLM model [17], exact solutions have been obtained for the particle kinetic stresses (velocity covariances) and the particle diffusion coefficients associated with an instantaneous point source located at the centre of the shear [32]. The results for the particle kinetic stresses are shown in Figures 2(a) as a function of the particle response time suitably normalized on the timescale of the turbulence which is homogenous and stationary (effectively the particle Stokes number St). x_1 is the streamwise direction and x_2 cross-streamwise direction. What is plotted is the difference between the streamwise and cross-streamwise components for the normal stresses normalized on $S^2 \langle u'^2 \rangle$ where S is the strain rate normalized on the time scale of the turbulence. What is noticeable is the difference is positive and it increases with Stokes number. As the particles cross the shear they extract turbulent energy from the mean flow – it's the work done by shear stresses in the streamwise direction which appears as an increase of turbulent kinetic energy in the streamwise direction. The second graph in Figures 2(b) is even more revealing. A calculation is made of the diffusion coefficients ϵ_{ij} which relate the diffusion current j_i to the gradients of the concentration gradient i.e.

$$j_i = \langle u_i \rangle \langle \rho \rangle - \epsilon_{ij} \frac{\partial}{\partial x_j} \langle \rho \rangle \quad (21)$$

Here we see the particle current composed of a convective term proportional to the local mean carrier flow and a long term a diffusive current. What is most interesting is the particle diffusion coefficient in the streamwise direction compared to that in the cross-streamwise direction. We note that for all Stokes numbers it is *-ve*, which includes that for a passive scalar! This does not imply however that contrary to the Second Law that a blob of particles will always contract rather than expand? These diffusion coefficients make a small contribution to the way a blob will diffuse. Particles will diffuse in the streamwise direction because as they move upwards or downwards they will experience larger positive or negative velocities according to how far away they are away from the origin. And that displacement is randomly positive or negative because it is determined by dispersion in the cross streamwise direction. So it is this process that makes the blob stretch in the streamwise direction. The *-ve* diffusion coefficients reduce this process but never reverse it. Figure 3 shows a picture of the concentration contours and the mean particle velocities at a time \sim integral times after they were released from the centre of the shear where the mean velocities are almost radial and later where they have rotated to align with the velocities of the shear during which time the contours have expanded.

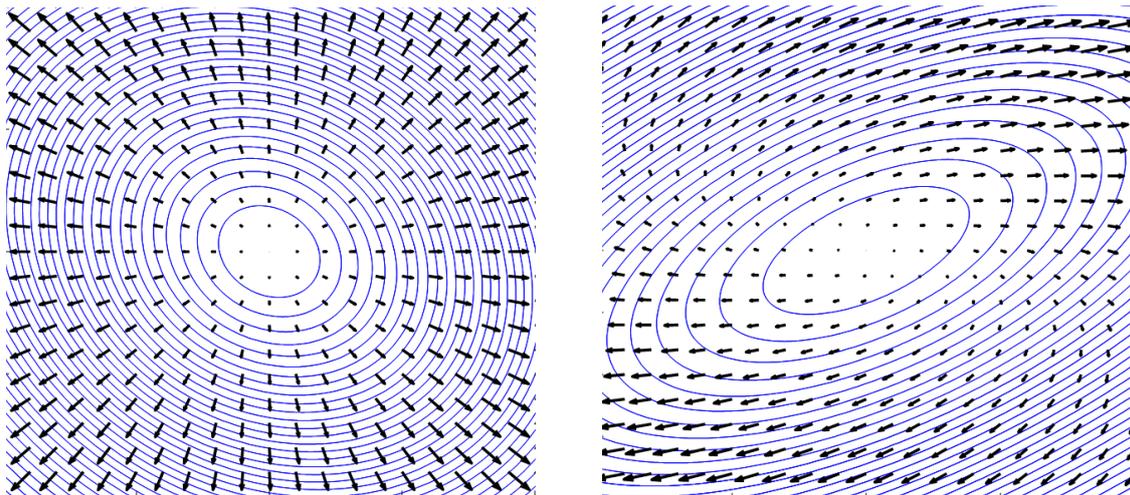
4. Transport and deposition in turbulent boundary layers

There has been intensive research over the last 20 years on the near wall behaviour of particles suspended in a turbulent flow (see e.g. recent review by Li and Ahmadi [23]), in particular how particles interact with near wall structures and how this transports and deposits them at the wall. In this regard DNS has been particularly useful in simulating the behaviour of the fluid motion. Much of our understanding comes from particle tracking in these flows. Of particular note is the work of Soldati and his co workers [37] in illuminating the transport mechanisms and in developing models for the particle deposition which has been the major preoccupation from a practical point of view. The problems here have been in formulating an appropriate transport equation to account for the influence of the severe changes in the turbulence intensity



a) Particle covariance (kinetic stresses) b) Long time particle dispersion coefficients ϵ_{ij}

Figure 2. Dispersion of particles in a simple shear based on Pope’s GLM versus Stokes number β^{-1} S is the strain rate normalised on turbulence integral time scale versus Stokes number β^{-1} . In the graphs $\epsilon_{ij} = \langle v_i'' x_j \rangle$



a) short term dispersion b) Long term dispersion

Figure 3. Concentration contours and particle mean velocity $St = 1$, normalised strain rate $S = 1$, at (a) $t = 1$ (b) $t = 6$ where t is in units of the integral timescale. Concentration contours represent a constant fraction f of the concentration at the centre of the shear, $f = 1 = 0.02n$, $n = 1, 2, \dots, k$

in the near wall region which in general makes the particle transport entirely non local, i.e. far from local equilibrium. In this regard the PDF approach has been particularly successful. Whilst the two-fluid equations are inappropriate near the wall, the solution of the PDF equation itself still provides a valid description. Furthermore the boundary conditions arising from the particle wall interactions are only expressible in terms of boundary conditions for a PDF equation since they involves changes in the velocity distribution at the wall. Traditional-fluid modelling is inappropriate because the boundary conditions (bc’s) imposed are artificial. We note that advection diffusion models for deposition are implicit in the particle momentum equation derived from the PDF equations where the inertial term is ignored [30].

$$j = \langle \rho \rangle v_d - \epsilon \cdot \frac{\partial \langle \rho \rangle}{\partial \mathbf{x}} \quad (22)$$

where

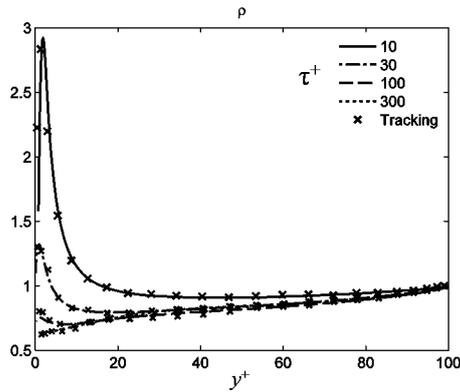
$$v_d = -\tau_p \frac{\partial}{\partial \mathbf{x}} \cdot \langle \mathbf{v}\mathbf{v} \rangle + \kappa - \frac{\partial}{\partial x} \cdot \boldsymbol{\lambda} \quad (23)$$

The drift velocity v_d is composed of essentially of two terms that are of different origin. The first term arises from the gradients of the kinetic stress and reflects a balance between a drag force and the gradients of a stress, whilst the remaining terms are derived from body forces that arise directly from spatial inhomogeneous in the flow. The first term has often been referred to as turbophoresis [27]. For precise details on the application of the PDF approach to near wall behavior and the influence of natural boundary we refer to the works of Devenish et al. [12], Reeks and Swailes [33] and Darbyshire and Swailes [10].

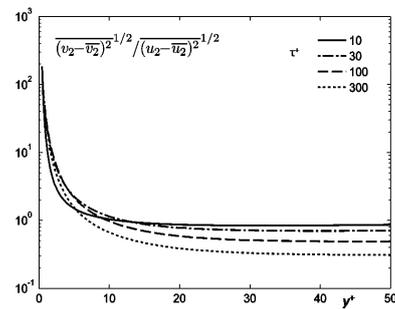
4.1. Particle deposition in turbulent boundary layers

Deposition of particles in turbulent pipe flow has a huge literature associated with it (see [23]) - there have been many attempts at predicting the deposition as a function of particle size or response time. The problem as we have seen is the rapid decay of turbulence near the wall and the way the particles respond to that decay and the lack of local equilibrium with the flow. The particles may start out in local equilibrium far away from the wall but their inability to follow the steep changes in the fluid velocity means that at any point the particles have some memory of their previous history - their velocity has more to do with where they came from than what is happening to the fluid motion locally. The continuum equations break down. Not only that, we have to deal with the problem of boundary conditions (bc's) if we use continuum equations because perfect absorption at the wall means that the only boundary conditions is that there are no particles at the wall with velocities away from the wall. There is no means of fitting that behaviour into a traditional no slip at the wall boundary condition. PDF equations are ideally suited for this type of problem - they take account of the natural bc's and secondly they take account of the influence of particle inertia and the steep turbulence gradients. They uniquely handle both effects together which traditional models are incapable of doing. It is useful to show some features of the near wall behaviour before considering what the deposition looks like. The results are taken from the recent analysis of vanDijk and Swailes [42] based on solution of the GLM PDF model using a discontinuous Galerkin method of solution. The Figure4(a) shows the concentration ratio as a function of distance y^+ from the wall (denoted by x_2 in the Figure 4) for a range of values of the particle inertia or particle response time in wall units τ^+ equivalent to the Stokes number. You can see a significant peaking of the concentration near the wall as τ^+ reduces from very large values where the motion is basically ballistic (no response at all to the near wall turbulence). Figure4(b) shows the ratio of the rms of the particle wall normal velocities, v_2 to local fluid rms of the fluid u_2 as a function of distance from the wall, indicating that this ratio $\gg 1$ as you approach the wall because of the particles' inertia and the much higher velocities they have attained further away from the wall where the gradients of the turbulence are much less.

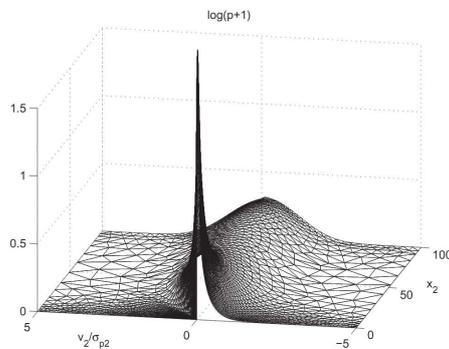
Figure 4(c) for the particle pdf $p(v_2, x_2)$ shows that particles enter the domain at $x_2 = 100$ for $v_2 < 0$, and subsequently move towards the wall via, mainly, a diffusive mechanism; the pdf remains close to the local equilibrium state over a large part of the spatial domain. Closer to the wall, at about $x_2 = 20$, the fluid rms velocity decreases rapidly. The effect of this is that the particles are no longer driven by diffusion, but start moving in free flight. Most of the heavy particles ($\tau^+ = 300$, see Figure 4) have enough momentum to reach the wall, even those that have a relatively low speed. Only very slowly moving particles get trapped near the wall, and slowly drift towards adhesion at $x_2 = X_0$. This results in a small build-up near the



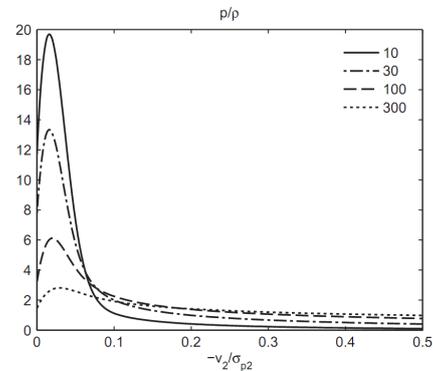
a) near wall particle concentration ρ



b) near wall particle normal rms normal velocities



c) near wall pdf $p(v_2, x_2)$ for $\tau^+ = 10$



d) particle velocity distribution for $\tau^+ = 10$ at 'wall' (one particle radius from wall).

Figure 4. Particle near wall behaviour as a function of distance from wall y^+ and particle response time τ^+ (both in wall units), van Dijk and Swailes [42] σ_{p2} is the local particle equilibrium rms velocity in the wall normal direction.

wall of particles with low velocity. For lighter particles ($\tau^+ = 10$, Figure 4(c)) only the fast particles reach the wall in free flight while most will be trapped. Hence the very sharp peak in the pdf around zero particle velocity. This feature that would not be picked up in the particle tracking because of the requirement of a very high resolution. This results in a strong build-up in concentration which is also clearly visible in Figure 4(a), where the particle concentration, ρ , in the boundary layer is shown. In fact recent work suggests that there is threshold velocity of τ^+ below which particles are trapped in the region of almost stagnant fluid near the wall and never get deposited (see the recent analysis of Sikovsky [35]). Similar features have been observed in particle pair collisions in homogeneous isotropic turbulence [16]. The normalised particle velocity distribution, is presented in Figure 4(d), illustrates this process as well: the distribution for $\tau^+ = 300$ has a significant tail, while for $\tau^+ = 10$ the distribution is strongly localised near $v_2/\sigma_{p2} = 0$.

Finally Figure 5 shows the predictions of the particle depositions velocity as a function of particle response time τ^+ obtained by Zaichik[49] compared to a range of experimental and DNS results. In particular Zaichik's predictions were obtained by solving a closed set of moment equations derived from the PDF kinetic equation. The closure is based on a quasi-normal assumption for the fourth-order moments of particle velocity and local-equilibrium closure for

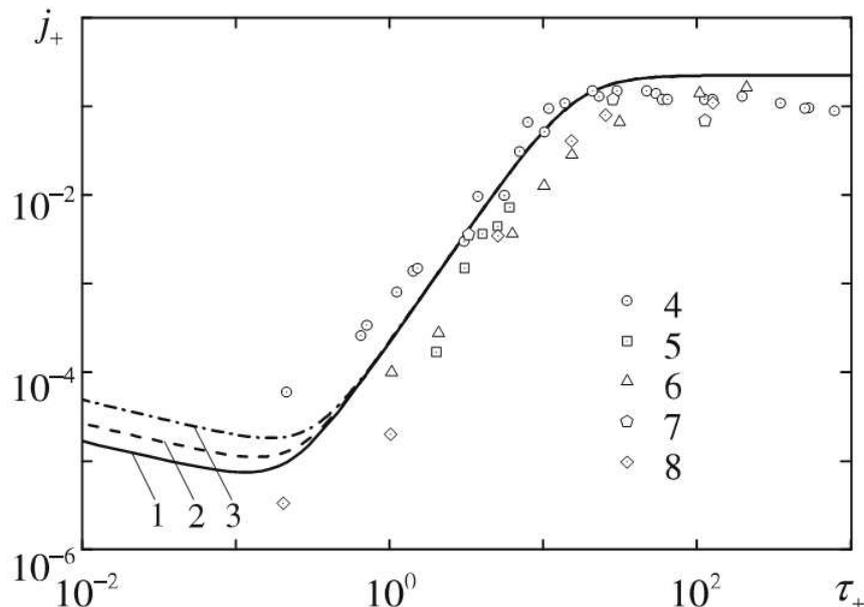


Figure 5. Particle deposition in turbulent pipe flow Zaichik [49]

3-rd order moments (neglecting their advection). The method of solution has thus much in common with the RANS approach in CFD involving Reynolds stress transport equations. Given the experimental error is very large the PDF solutions predicts the huge changes in deposition velocity from 10^{-1} to 10^{-5} for a change in τ^+ from 10 to 10^{-1} which reflects the role of particle inertia on the deposition.

5. Segregation and Agglomeration

It is by now well known that turbulence, contrary to traditionally held views, can demix a suspension of particles (see e.g. [14]). The process of segregation depends upon the ratio of the particle response time to the timescale of the turbulent structures in the flow (i.e the Stokes number, St). Early experiments and simulations (e.g. [9]) have shown that the demixing reaches a maximum when the particle response time is approximately equal to the timescale of the turbulent structure (i.e the particle Stokes number $St \sim 1$), the suspended particles being observed to segregate into regions of high strain rate in between the regions of high vorticity. This feature is best illustrated graphically in Figure 6 which shows the segregation patterns arising from a point source of particles diffusing in a 2-D random array of counter rotating vortices. The Figure shows the segregation pattern at a given value of time (in units of the integral time scale) after the source has been introduced into the flow for 3 values of the particle Stokes number $St = 0.05, 0.5, 5$. It is clear that maximum segregation occurs for the case of $St = 1$. What this Figure doesn't show however is the fact that the segregation continues in time, the patterns becoming more filamental. Whatever their Stokes number all particles will segregate, it is just that the greater the Stokes number the longer the process takes to achieve a given level of segregation. This is contrary to what many have thought that the segregation reaches an equilibrium state. Particles will segregate until they touch. In fact what happens is that the segregation forms a network of filamental *caustics* similar to the patterns of light obtained at the bottom of swimming pools as shown in Figure 6(d) where within these filamental networks it is observed that the light beams cross one another. Similarly in the case of particle segregation in a turbulent flow within the filamental caustics particle trajectories are observed to cross also. The formation of caustics in particle demixing processes was first

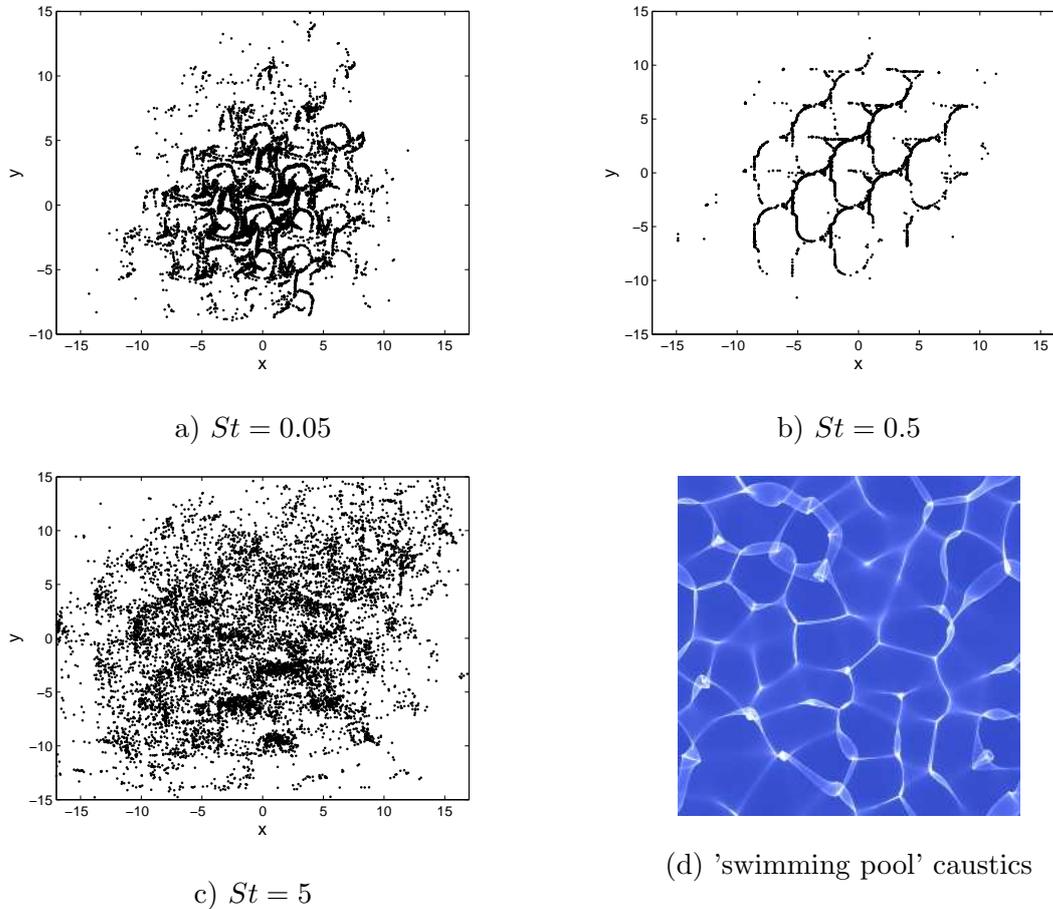


Figure 6. Segregations as a function of particle Stokes number St (a)-(c) based on positions of 10^4 particles after time $t = 20$ in a non-isotropic random straining flow, (d) caustic patterns observed at the bottom of a swimming pool.

recognised by Wikinson and Mehlig [45] and this crossing of trajectories within a caustic is intimately related to the occurrence of random uncorrelated motion (RUM) in flow fields that are spatially random but smoothly varying. Fevrier, Simonin & Squires [15] have observed that the spatial particle velocity field resulting from the motion of suspended particles in a direct numerical simulation (DNS) of homogeneous isotropic turbulence consists of two components: a smoothly (continuous) velocity field that accounts for all particle-particle and fluid-particle two point spatial correlations (they referred to this component as the mesoscopic Eulerian particle velocity field (MEPVF)); and a spatially uncorrelated component which we have referred to as RUM (the component of random uncorrelated motion) whose contribution to the particle kinetic energy increases as the particle inertia increases. Fevrier, Simonin & Squires attribute this feature to the ability of the particles with inertia to retain the memory of their interaction with very distant, and statistically independent eddies in the flow field.

Segregation and RUM are related to the occurrence of inter-particle collisions as follows from the seminal work of Sundaram and Collins [40] and Wang and Wexler [43] in which they demonstrate that i) segregation enhances the particle concentration of certain regions of the flow, ii) RUM, i.e. the decorrelation of velocity between particles, causes two nearby particles to collide and possibly to agglomerate. Segregation is well-known to manifest itself especially for $St \sim 1$, whereas the effect of RUM is almost invisible for small particles and becomes increasingly

important for larger St . Since the interplay between these two effects determines the collision rate in a turbulent flow, it is essential to quantify segregation and RUM as accurately as possible as a function of the Stokes number and some typical flow properties in order to correctly predict the rate of inter particle collisions.

In recent years, the process of segregation of inertial particles has been studied from different viewpoints when the Stokes number is relatively small. On the one hand, [7] demonstrated a strong correlation between the positions of small inertial particles and the locations of zero-acceleration points in the carrier flow. On the other hand, [1] carried out a theoretical analysis based on the assumption that the velocity of inertial particles can be directly related to the carrier flow velocity. By doing so, they were able to show that the segregation of particles continues indefinitely in the course of time, and they showed that the concentration of inertial particles in a turbulent flow is highly intermittent, so the particles are distributed far from uniformly over space. A similar approach was chosen by Chun et al. [8] who demonstrated that the time-converged solution of the radial distribution function is of the form $g(r) \sim r^\beta$, where the negative number β is proportional to St^2 . In addition, they confirmed this by showing results from a DNS of statistically stationary homogeneous isotropic turbulence. Most importantly the PDF/ kinetic approach has been used by Zaichik ([47] [48]) to obtain a similar result.

The understanding of dilute suspensions of inertial particles has been vastly extended by interpreting the motion of particles in terms of dynamical systems theory. The first approach in this direction was given by [38], and was later specifically applied to the motion of inertial particles in turbulent flows by [2] and [45]. [45] derived an analytical expression for the Lyapunov exponents associated with the motion of inertial particles in physical space. The derivation was based on the assumption that the typical correlation time of the carrier flow was very small, i.e. the Kubo number $Ku \ll 1$. Unfortunately, this assumption is not exactly valid in real turbulence where $Ku = \mathcal{O}(1)$, as [45] acknowledge themselves. [2] showed that if the particle clustering is fractal, the exponent in the radial distribution function is equal to $\beta = n_d - D_{corr}$, where D_{corr} is the correlation dimension introduced by [19], and n_d is the number of dimensions of the problem ($n_d = 2$ in a two-dimensional flow and $n_d = 3$ in a three-dimensional flow). [2] expressed the clustering of particle in terms of its fractal dimension in phase space and showed how this was related to the Lyapunov exponents of the $2n_d$ -dimensional dynamical system. [3] obtained a correlation dimension D_{corr} by calculating the Lyapunov exponents in a Direct Numerical Simulation of turbulence for a wide range of Stokes numbers, and found that $n_d - D_{corr}$ scales with St^2 , in agreement with the aforementioned results by [8].

We will describe now how a particular method known as the Full Lagrangian Method (FLM) has been used very effectively to investigate the statistics of particle segregation in both DNS and in synthetic turbulence flows like those produced in kinematic simulation (KS). This method, originally introduced by [25] but later used by [31] and [18], consists of calculating the size of an infinitesimally small volume occupied by a group of particles, along the trajectory of one single particle. This immediately yields the concentration of particles along the trajectory, since the inverse of the volume occupied by a fixed number of particles corresponds to the particle concentration by definition. We describe how the results from the FLM are converted into statistics of the particle number density, thus providing a wealth of information on the segregation process. In particular we describe here how the FLM can be used to quantify non-uniformities in the spatial distribution of particles, the singularities in the particle concentration field and the presence of RUM.

5.1. The Full Lagrangian Approach

We consider small spherical particles acted on by Stokes drag for which the equation of motion of each particle is given by

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \quad ; \quad \frac{d\mathbf{v}}{dt} = \frac{1}{St}(\mathbf{u} - \mathbf{v}) \quad (24)$$

where \mathbf{x} and \mathbf{v} denote the position and the velocity of the particle, respectively, $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$ is the velocity of the carrier flow at the position of the particle and St is the particles Stokes number. FLM calculates the deformation of an elemental volume of particles as it moves through the flow. The deformation of such a volume is characterized by the temporal evolution of the unit deformation tensor \mathbf{J} , whose components J_{ij} are defined by:

$$J_{ij} \equiv \frac{\partial x_i(\mathbf{x}_0, t)}{\partial x_{0,j}}, \quad (25)$$

where \mathbf{x}_0 is the position of the particle at some initial time say $t = 0$. Differentiating Eq. 25 with respect to time gives:

$$\frac{d}{dt} J_{ij} = \frac{\partial v_i(\mathbf{x}_0, t)}{\partial x_{0,j}}. \quad (26)$$

$$\frac{d}{dt} J_{ij} = \frac{\partial v_i(\mathbf{x}_0, t)}{\partial x_{0,j}}. \quad (27)$$

The second derivative with respect to time is:

$$\frac{d^2}{dt^2} J_{ij} = \frac{\partial}{\partial x_{0,j}} \left(\frac{dv_i(\mathbf{x}_0, t)}{dt} \right) = \frac{1}{\tau_p} \left(\frac{\partial x_k}{\partial x_{0,j}} \right) \frac{\partial}{\partial x_k} u_i(\mathbf{x}, t) - \frac{1}{\tau_p} \frac{\partial v_i(\mathbf{x}_0, t)}{\partial x_{0,j}}. \quad (28)$$

Inserting Eq. 25 and Eq. 27 into Eq. 28 results in the equations of motion of each component J_{ij} :

$$\frac{dJ_{ij}}{dt} = \dot{J}_{ij}, \quad \frac{d}{dt} \dot{J}_{ij} = \frac{1}{\tau_p} \left(J_{kj} \frac{\partial u_i}{\partial x_k} - \dot{J}_{ij} \right), \quad (29)$$

We choose as initial conditions $J_{ij}(0) = \delta_{ij}$ and $\dot{J}_{ij}(0) = \partial u_i(\mathbf{x}_0, 0)/\partial x_j$. The volume expansion $J(t) = |\det J_{ij}|$. If the initial distribution of particles is uniform over a certain domain, the deformation in the course of time is inversely proportional to the particle number density $n(t)$ measured along the trajectory of one reference particle is related to J by

$$J = n^{-1}(t) \quad (30)$$

Thus a spatially averaged moments of the particle number density, n , can be calculated directly from the deformation \mathbf{J} along sufficiently many particle trajectories.

5.2. The Statistics of the compression

The Full Lagrangian Method can thus be used to determine the compressibility of the particle phase, \mathbb{C} which we define as $J^{-1}dJ/dt = d \ln J / dt$. We can relate this to the divergence of the particle velocity field $\mathbf{v}_p(\mathbf{x}, t)$ providing that the velocity field is single valued and continuous, namely

$$\mathbb{C} = d \ln J / dt = \nabla \cdot \mathbf{v}_p(\mathbf{x}, t)$$

We present some results based on the FLM for a 'kinematic' flow field composed of 200 random Fourier modes (referred to as kinematic simulation (KS)) [22][24]. In addition we also present the statistics of the particle number density and the contribution that RUM makes to the kinetic energy of the transported particles. Fig. 7 shows the results of $\lim_{t \rightarrow \infty} t^{-1} \langle \ln |J| \rangle$ for

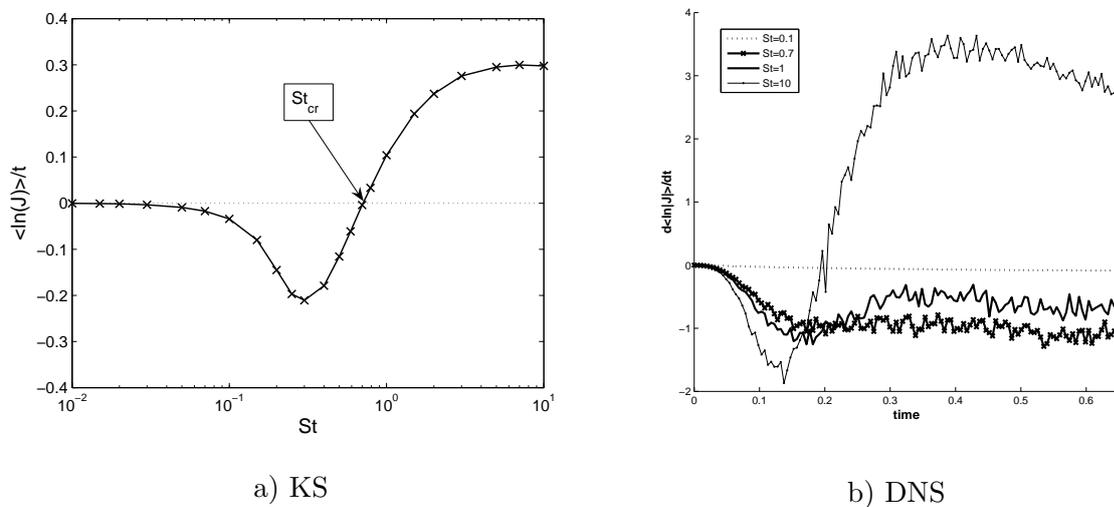


Figure 7. Long term net compressibility as a function of time in flow field composed of random Fourier modes (KS) and DNS of homogeneous isotropic turbulence

a wide range of values of Stokes numbers. It is noted that this value is equal to $\lim_{t \rightarrow \infty} \langle C \rangle$, i.e. the time converged compressibility of the particle velocity field. We note that there is a critical value of the Stokes number St_{cr} beyond which the net compressibility is positive rather than negative.; in the present case, $St_{cr} \simeq 0.7$. If the particle Stokes number St is lower than St_{cr} , then the particles are continuously compressed into smaller volumes in the course of time and the process of segregation continues indefinitely. If, on the other hand, the Stokes number is larger than St_{cr} , the particle volumes expands or alternatively if the particles are confined they become fully mixed. This doesn't mean that there is no segregation beyond the critical Stokes number. It is clear that an average quantity only provides us with a picture of the net effect between compression/expansion and what effect prevails in the course of time: a compressibility – on average – does not necessarily mean that the segregation is zero everywhere. The same applies to negative compressibility. Indeed, the sign of the compressibility can be related to the topological distribution of the particle concentration field: as particles cluster, compression zones appear (in the clusters) at the same time as dilation zones (in the depleted zones).

5.3. Statistics of the particle number density

Now we investigate the statistics of the particle number density in the course of time. The moments of the particle number density \bar{n}^α have been determined for both the KS and DNS flow fields. The results are shown in Figure. 8, for (a) $St = 0.05$ (b) $St = 0.5$ in the case of the KS flow field and in (c) for $St = 0.4$ for a DNS flow field. In all cases the value of \bar{n}^0 , which corresponds to $\langle |J| \rangle$, remains equal to unity for all time, as expected. The other moments of the particle number density are markedly higher than 1 and are associated with the non-uniformity in the spatial distribution of particles.

There is a qualitative distinction between the cases of small Stokes numbers such as $St = 0.05$ in Fig. 8 a), and large Stokes numbers such as $St = 0.5$ in Fig.8 b). If the Stokes number is large, it may happen that $|J| = 0$ for a particle due to the crossing of trajectories. These intermittent events, which cause $n \rightarrow \infty$, dominate the statistics of higher-order moments of the PDF at certain moments in time, as is reflected by the spikes in the curve for $St = 0.5$ in Fig. 8b). Hence, the spatial distribution of particles in a random turbulence-like flow may be highly intermittent. This is also the case for the DNS moments in Figure 8(c)

However, for sufficiently small Stokes numbers where RUM is not important (such as $St = 0.05$ in Fig.8 a)), we observe that $\overline{n^\alpha}$ depends exponentially on time and:

$$\overline{n^\alpha} \propto \exp(\gamma t), \quad (31)$$

where γ is a function of α and St . As can be seen in a), the higher-order moments grow faster than the lower-order moments. This demonstrates unambiguously that the segregation process continues indefinitely in this case where $St = 0.05$.

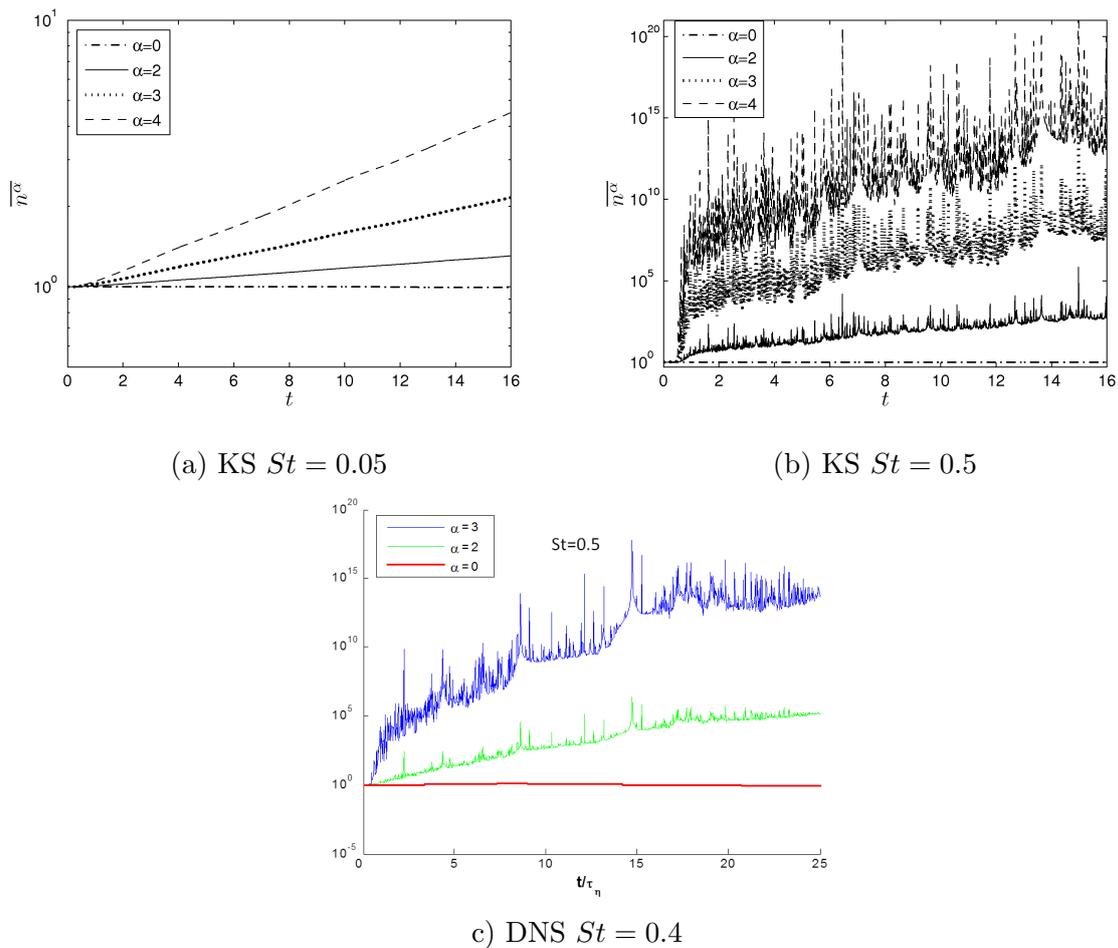
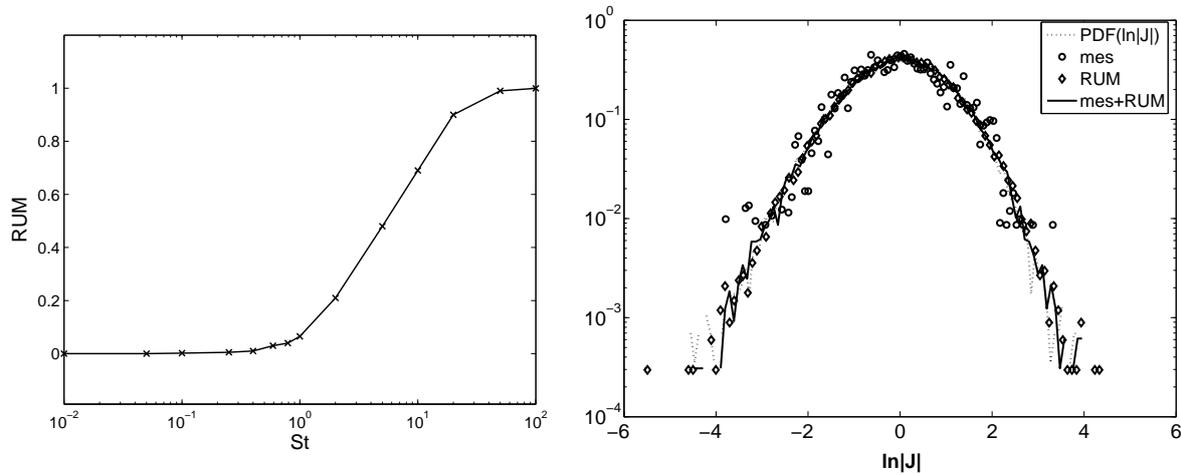


Figure 8. Spatially average of the α -th moment of the particle number density, $\overline{n^\alpha}$, for KS flow field a) $St = 0.05$; b) $St = 0.5$ (c) DNS $St = 0.4$

Random uncorrelated motion (RUM)

We present here results for the contribution RUM makes to the kinetic energy of the particles transported in a KS generated carrier flow field. The values are obtained by measuring the longitudinal velocity correlation between two particles separated by a distance r . Extrapolation of the correlation to $r = 0$, gives an intercept for which the RUM contribution is 1 - this quantity. The RUM contribution to the kinetic energy is shown in Figure 9(a) as a function of the particle Stokes number St . We note that for $St \rightarrow 0$, the RUM contribution $\rightarrow 0$ whilst for $St \rightarrow \infty$, it \rightarrow unity i.e totally ballistic motion.

Figure 9(b) show the distribution of the fluctuating value of the compression \mathbb{C}' normalised on its rms value obtained by Meneguz and Reeks [24]. Each value of \mathbb{C}' has been separated



a) RUM contribution to particle kinetic energy

b) $P(\mathbb{C})$, $\mathbb{C} = \ln J$

Figure 9. RUM contribution to (a) particular kinetic energy as a function of Stokes number St and to (b) distribution P of compression \mathbb{C} . Both cases refer to the flow field composed of random Fourier modes.

out into its RUM components and its smoothly varying mesoscopic component. We note that negative values of \mathbb{C}' in the extreme range, are almost entirely made up of the RUM uncorrelated component which is consistent with the formation of caustics of high regions of segregation and concentration.

The results presented here show that particle inertia can have major implications for the collision rates between particles. Two effects enhance the collision rate between particles: i) preferential concentration of particles in relatively few regions of the flow, ii) RUM, i.e. the decorrelation of velocities between neighboring particles so that particles are more likely to collide with one another. From Fig.7, we know that preferential concentration manifests itself especially for $0.1 < St < 1$. The effect of RUM is most visible for $St > 0.5$ and increasingly important for larger St . Collision rates are therefore expected to be highest in the Stokes number regime $St > 0.5$. Certainly more research is needed to confirm this statement, but the results presented in the seminal paper by [40] do point in that direction, since they found a maximum collision rate for a Stokes number St (based on the smallest scale of the flow, the Kolmogorov time scale) of $2 < St < 5$, with a collision rate vanishing for $St \downarrow 0$, and a collision rate decreasing only slowly with St if $St > 5$.

6. Summary and Conclusions

This paper describes methods and approaches that have been used to simulate and model the transport, mixing and agglomeration of small particles in a flowing turbulent gas (referred to as *turbulent aerosols*). The transported particles because of their inertia are assumed not to follow the motion of the large scales of the turbulence (referred to as one point particle dispersion) and or the motion of the small dissipating scales of the turbulence (referred to as two point particle or relative dispersion). The major studies of one point particle transport have been associated with developments in two-fluid modelling where the particles are treated as a fluid in the same way as the carrier flow. The purpose has been to find suitable forms for the continuum equations of the dispersed particle phase together with the constitutive relations. The objective has been to model complex dispersed flows using much the same approach as in CFD for single phase flow. Of great value in this approach has been the application of the PDF approach involving

a Master Equation analogous the Maxwell-Boltzmann equation of Classical Kinetic Theory. In this paper we looked at two PDF approaches, a kinetic approach which is concerned with the probability that a particle has a certain velocity and position and an alternative approach which considers an extra random variable, namely the carrier flow velocity measured by the particle along its trajectory. It was referred to as the GLM approach because the equation of motion for this flow velocity is based on a Generalized Langevin model (GLM) used by Pope [17]. We have described the success of these approaches in modelling simple generic flows and transport of particles in a turbulent boundary layer.

The work reported on two particle dispersion has been about methods of measuring and analyzing the statistics of particle segregation. In particular we have described the Full Lagrangian Method (FLM) which measures the deformation of an elemental volume of particles as it moves through the fluid along a particle trajectory. The statistics of the segregation process has been described in terms of the statistics of the compressibility which is shown to have a mean component and a fluctuating which is close to Gaussian except in the wings where the existence of singularities contributes to extremely large values of negative compression and the moments of the particle concentration. We have shown that these features are all compatible with the formation of caustics.

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