Particle drift in turbulent flows: the influence of local structure and inhomogeneity

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Abstract

The way particles interact with turbulent structures, particularly in regions of high vorticity and strain rate, has been investigated in simulations of homogeneous turbulence and in simple flows which have a periodic or persistent structure e.g. separating flows and mixing layers. The influence on both settling under gravity and diffusion has been reported and the divergence (compressibility) of the underlying particle velocity field along a particle trajectory has been recognized as an important quantity in quantifying these features. This paper shows how these features can be incorporated in a formal way into a two-fluid model of the dispersed particle phase. In particular the PDF equation for the particle velocity and position is formally derived on the basis of a stochastic process that involves the statistics of both the particle velocity and local compressibility along particle trajectories. The PDF equation gives rise to contributions to both the drift and particle diffusion coefficient that depend upon the correlation of these quantities with the local carrier flow velocity.

Key Words: turbulent structures, particle dispersion, drift, PDF approach

1. INTRODUCTION

There are two aspects of the motion of particles in turbulent flows that have not been properly incorporated in a rational way into a two-fluid model of a dispersed particle flow, namely the influence of persistent structures in the underlying carrier flow, and the occurrence of drift (either under the influence of gravity or as a result of inhomogeneity in the underlying turbulence). In their numerical simulations of particle settling in homogeneous turbulence and in cellular flow fields, Maxey and his co-workers have shown for instance that turbulence can enhance the settling of small particles, (Maxey & Corrsin 1986, Maxey 1987, Wang & Maxey 1993). In particular Maxey (1987) showed that in situations of weak particle inertia (i.e. particle relaxation times \( \ll \) the typical time scale of the turbulent structures in the flow) the net settling velocity \( \mathbf{V}_g \) of an ensemble of particles in a homogeneous flow field was related to its value \( \mathbf{V}^0_g \) in quiescent flow by the relationship

\[
\mathbf{V}_g = \mathbf{V}^0_g - \int_0^t \langle \mathbf{u}(\mathbf{x}, t) \nabla \cdot \mathbf{v}_p(X_p(\mathbf{x}, t | s), s) \rangle \, ds,
\]

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where $\langle \ldots \rangle$ is an ensemble average; $\mathbf{u}(\mathbf{x}, t)$ is the carrier flow turbulent velocity field at position $\mathbf{x}$ for times $t \gg$ integral time scale of the turbulent motion; $\nabla \cdot \mathbf{v}_p(\mathbf{X}_p(\mathbf{x}, t | s), s)$ is the divergence of the particle velocity field $\mathbf{v}_p(\mathbf{y}, s)$ with respect to the spatial position $\mathbf{y}$ measured at $\mathbf{y} = \mathbf{X}_p(\mathbf{x}, t | s)$ at time $s$ where $\mathbf{X}_p(\mathbf{x}, t | s)$ is the position of a particle at $s$ which arrives at $\mathbf{x}$ at time $t$. The particle velocity field $\mathbf{v}_p(\mathbf{y}, t)$ is defined as the particle velocity field arising from one realisation of the flow field $\mathbf{u}(\mathbf{y}, t)$ with a prescribed set of initial conditions at $s = 0$ for the particles which are the same in each realisation of the flow field.

The divergence of the particle velocity field is a measure of the local compressibility of the particle flow. The presence of gravity means that the particles move in a preferential direction which in turn means that the correlation of the fluid velocity with the ‘local’ divergence of the particle flow field is non-zero. For the case when the particles almost followed the flow, Maxey was able to relate the local compressibility of the particle flow field to the local straining of the underlying carrier flow and showed that the value of the correlation would lead to an enhancement of the gravitational settling. Subsequently Wang & Maxey (1987) explained this result in more detail by looking at the way particles move around the edges of vortices; in particular their results could be explained by the streaming of particles between vortices which always lead to an accumulation of particles on the down flow side of vortices (i.e. in the direction of gravity). They referred to this process as preferential sweeping. This however is not a unique result. For instance depending upon the particle Froude number, Davila and Hunt (1999) have shown it is possible for the opposite to occur.

Whatever the particular route the particles take through a flow field (with or without gravity), the compressibility of the particle flow field measured along a particle trajectory is an important consideration in the way we assess the influence of structures. The work presented here shows that Maxey’s expression for the drift is a much more general result appropriate for inhomogeneous as well as homogeneous flows with or without the presence of gravity. Indeed it is shown that the compressibility of the particle flow can influence not only the drift but also the particle dispersion. As a prelude to the full two-fluid formulation I first consider in Section 2 the analysis of particle dispersion and drift in a compressible flow field in which the statistics of both the particle velocity and the divergence of the particle flow field along a particle trajectory are prescribed and correlated. Then finally in Section 3 these features are incorporated into a two-fluid model of the dispersed particle phase, based on the so-called pdf approach - the focus here being on the derivation of the appropriate transport equation for the particle phase space probability that a particle has a velocity $\mathbf{v}$ and position $\mathbf{x}$ at time $t$. Some of the features of this analysis are illustrated in particle dispersion in a random array of counter-rotating vortices in both homogeneous and inhomogeneous situations depending upon the prescribed statistics.

2. PASSIVE SCALAR DISPERSION IN A COMPRESSIBLE FLOW

2.1 Gaussian and non-Gaussian Lagrangian Statistics

Analyses of this sort have been done before for passive scalar diffusion in incompressible flow in which case only the statistics of the particle velocity along a particle trajectory are required. In the case of a compressible flow, moments associated with the process
[\mathbf{v}_p(s), \nabla \cdot \mathbf{v}_p(s), s \in t] appear as a natural consequence of the transport and the compressibility of the flow, where both the particle velocity and the divergence of the particle velocity fields are measured along a particle trajectory.

The starting point of the analysis is the conservation equation for the particle mass density \( \rho(\mathbf{x}, t) \) at position \( \mathbf{x} = [x_1, x_2, x_3] \) at time \( t \), namely

\[
\frac{\partial \rho}{\partial t} = -\nabla \cdot \{ \mathbf{v}_p \rho(\mathbf{x}, t) \},
\]

or

\[
\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}_p(\mathbf{x}, t). \tag{2}
\]

where is \( D/Dt \) rate of change along a particle trajectory. Given some initial distribution \( \rho(\mathbf{x}, t_0) \) at time \( t = 0 \), the solution is formerly

\[
\rho(\mathbf{x}, t) = \rho \left( \mathbf{x}_p(\mathbf{x}, t|0), 0 \right) \exp \left\{ -\int_{t_0}^{t} \nabla \cdot \mathbf{v}_p(\mathbf{x}_p(\mathbf{x}, t|s), s) \, ds \right\}. \tag{3}
\]

where \( \mathbf{x}_p(\mathbf{x}, t|s) \) is the position at time \( s \) of a particle arriving at \( \mathbf{x} \) at time \( t \). Given that in principle we can define a particle velocity field \( \mathbf{v}_p(\mathbf{x}, t) \) for any realization of the underlying carrier flow field, then the problem of particle dispersion and settling is identical to the problem of passive scalar dispersion in a velocity field differing only from the normal case considered in that the particle velocity field is compressible rather than solenoidal. Replacing \( \mathbf{X}_p(\mathbf{x}, t|0) \) by \( \mathbf{x} - \int_{t_0}^{t} \mathbf{v}_p(\mathbf{x}_p(\mathbf{x}, t|s), s) \, ds \) in Eq.(3) we obtain

\[
\rho(\mathbf{x}, t) = \rho \left( \mathbf{x} - \int_{t_0}^{t} \mathbf{v}_p(\mathbf{x}, t | s) \, ds, 0 \right) \exp \left\{ -\int_{t_0}^{t} \nabla \cdot \mathbf{v}_p(\mathbf{x}, t | s) \, ds \right\}. \tag{4}
\]

where \( \mathbf{v}_p(\mathbf{x}, t | s) \) and \( \nabla \cdot \mathbf{v}_p(\mathbf{x}, t | s) \) are used as shorthand notation for the explicit values of the particle velocity and divergence along particle trajectories that pass through \( (x, t) \) respectively.

\[
\mathbf{v}_p(\mathbf{x}, t | s) \equiv \mathbf{v}_p(\mathbf{X}_p(\mathbf{x}, t|s), s) \quad \nabla \cdot \mathbf{v}_p(\mathbf{x}, t | s) \equiv \nabla \cdot \mathbf{v}_p(\mathbf{y}, s)]_{y = x_p(\mathbf{x}, t|s)} \tag{5}
\]

We shall sometimes abbreviate these quantities still further to \( \mathbf{v}_p(\mathbf{s}) \) and \( [\nabla \cdot \mathbf{v}_p](\mathbf{s}) \) respectively. By making certain assumptions about the statistics of the process \( [\mathbf{v}_p(s), \nabla \cdot \mathbf{v}_p(s)] \) for \( 0 \leq s \leq t \), then we are avoiding the non-linearity of the diffusion process that is implicit in the relationship between Lagrangian and Eulerian timescales. As a result it is shown in Appendix A that if this process is jointly Gaussian then the particle drift velocity is given precisely by the term in Eq.(4) and the diffusion coefficient consistent with Taylor’s theory. Explicitly the particle mass current is given by:

\[
\langle \rho \mathbf{v}_p(\mathbf{x}, t) \rangle = \left\{ \langle \mathbf{v}_p(\mathbf{x}, t) \rangle - \int_{t_0}^{t} \langle \mathbf{v}_p(\mathbf{x}, t) \nabla \cdot \mathbf{v}_p(\mathbf{x}, t | s) \rangle \, ds \right\} \langle \rho(\mathbf{x}, t) \rangle
\]

\[
- \int_{t_0}^{t} ds \langle \mathbf{v}_p(\mathbf{x}, t) \mathbf{v}_p(\mathbf{x}, t | s) \rangle \cdot \nabla \langle \rho(\mathbf{x}, t) \rangle \tag{6}
\]

where \( \mathbf{v}_p(\mathbf{x}, t) \) is the fluctuating part of \( \mathbf{v}_p(\mathbf{x}, t) \) relative to its mean. The first bracketed term on the RHS (the drift term) in this equation is identical to the drift term derived by

\[2\text{It is implicit here that the divergence be applied to the spatial components of the particle velocity field and is not meant to operate on } \mathbf{x} \text{ in the vector function } \mathbf{v}_p(\mathbf{x}, t | s).\]
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Maxey if we substitute \( \mathbf{V}^0_p \) for \( \langle \mathbf{v}_p(x, t) \rangle \). However with the assumption that the statistics for the underlying particle velocity field are Gaussian, we end up with a more general result which includes a gradient diffusion flux. If in general the statistics of the process \( [\mathbf{v}_p(t), \nabla \cdot \mathbf{v}_p(t)] \) are non-Gaussian then it is shown in Appendix A to first order in the triple moments of the process, that the particle mass current is compounded of a drift term

\[
\mathbf{v}_d = \langle \mathbf{v}_p(x, t) \rangle - \int_0^t ds \langle \nabla \cdot \mathbf{v}_p(x, t | s) \mathbf{v}_p'(x, t) \rangle + \frac{1}{2} \int_0^t ds_1 \int_0^t ds_2 \langle \mathbf{v}_p'(x, t) \nabla \cdot \mathbf{v}_p(x, t | s_1) \nabla \cdot \mathbf{v}_p(x, t | s_2) \rangle
\]

and a gradient diffusion term with diffusion coefficients \( D_{ij} \)

\[
D_{ij} = \int_0^t ds_1 \langle \mathbf{v}_p'(x, t | s) \mathbf{v}_p'(x, t) \rangle - \int_0^t ds_1 \int_0^t ds_2 \langle \mathbf{v}_p'(x, t) \mathbf{v}_p'(x, s_2) \nabla \cdot \mathbf{v}_p(x, t | s_1) \rangle
\]

2.2 Comments on the process \( [\mathbf{v}_p(s), \nabla \cdot \mathbf{v}_p; 0 \leq s \leq t] \)

It is important to recognize that the statistics of the process \( [\mathbf{v}_p(s), \nabla \cdot \mathbf{v}_p(s); 0 \leq s \leq t] \) which we will call \([q(s)]\) for short, does not depend on the initial concentration. If it did, then its statistics would be related to the particle density weighted averages we are trying to calculate in the first place. How these statistics are obtained is clear: a particle trajectory is solved backwards in time starting from \( x \) at time \( t \) using the values of the particle velocity \( \mathbf{v}_p(x) \) along its trajectory which in turn are derived from the statistics of the velocity field \( \mathbf{v}_p(x, s) \) where \( 0 \leq s \leq t \). No restrictions are placed on the point the trajectory goes through at time zero. In the actual problem of interest we might want to know the average particle velocity at \( x \) at time \( t \) knowing say that the particles started out at \( x_0 \) at time zero. So these particular particles will choose a particular subset of the statistics of the process \([q(s)]\) in arriving at \( x \) at time \( t \). That is, we are selecting only those trajectories of all those trajectories defined by the process \([q(s)]\) that go through \( x_0 \) at time zero from which we could compute the particles average velocity at \( x \) at time \( t \). Put another way, we are trying to evaluate the particle statistics from a set of statistics which are independent of where the particles start from in the actual problem of interest. You can see this more transparently in the way the concentration is calculated. You start off with some prescribed statistics for the process \([q(s)]\) found by starting a test particle off at \( x \) and solving the equation of motion backwards in time from \( t \). That is you solve

\[
\frac{dX_p}{ds} = \mathbf{v}_p(X_p, s) \text{ with } X_p(t) = x
\]

backwards in time to find the values of \( X_p(0) \)and the value of exponential of the integral of the value \( \nabla \cdot \mathbf{v}_p \) along a trajectory (which gives the fractional change in an elemental volume at time \( t \) along the trajectory relative to its initial value i.e. the value of the elemental volume deformation \( J(t) = \left[ \frac{\partial X_p(\omega, x, t)}{\partial \omega} \right] \)). You then calculate the concentration that particles would have at \([x, t]\) if they started out at time \( 0 \) with some concentration \( \rho(X_p(0), 0) \) by multiplying this concentration by \( J(t) \). If the concentration at \( X_p(0) \) happens to be zero, then the concentration at \( x \) is zero. The fact that there may not be any particles at \( X_p(0) \) doesn’t affect the statistics of the process \([q(s)]\). The process just tells
you where you might find some particles at time 0 but if there aren’t any, then that’s because of the initial conditions. The process \( q(s) \) doesn’t know about initial conditions or concentration. It’s entirely determined from the statistics of \( v_p(x, t) \) derived from some test particle at \( x \) at time \( t \) in the way we have prescribed.

2.2 Dispersion in homogeneous stationary turbulence and comparison with Taylor’s Theory

It is revealing to compare these results derived for passive scalar diffusion in a compressible flow field with G I Taylor’s classic theory for diffusion by continuous movements in a homogenous stationary flow field? We recall that Taylor’s results are based on the assumption that in the limit of the dispersion time \( t \to \infty \) this time can be divided into a large number of time steps (each step \( \gg \) the integral timescale of the turbulence) so that the distance travelled in one time step will be uncorrelated with the distance travelled in the next. This leads to Gaussian statistics for the particles displacement. In particular the diffusion coefficient is written as

\[
D_{ij} = \int_0^\infty R_{ij}(s) ds,
\]  

(10)

where \( R_{ij}(s) \) defines the velocity autocorrelation \( \left< v_{p_i}(x, 0 | s_1) v_{p_j}(x, 0 | s_2) \right> \) for which \( s = s_1 - s_2 \), and \( v_{p_i}(x, 0 | s_1) \) and \( v_{p_j}(x, 0 | s_2) \) as before are the velocities of a particle measured at time \( s_1 \) and \( s_2 \) that particle starting out at some arbitrary position \( x \) at some arbitrary time \( t = 0 \). The important requirement is the distances at which these measurements take place are on average very far away from the point of release \( x \) so that the process \( \left< v_p(x, 0 | s) \right> \) is stationary i.e for this to occur \( s/T_L \gg 1 \) where \( T_L \) is the Lagrangian integral timescale. The rate of change of the mean square displacement is given by

\[
\left[ \frac{d}{dt} \left< X_{p_i}(x, 0 | t)^2 \right> \right] = 2 \left< v_{p_i}(x, 0 | t) X_{p_i}(x, 0 | t) \right> = 2 \int_0^t \left< v_{p_i}(x, 0 | t) v_{p_i}(x, 0 | s) \right> ds
\]

(11)

and with the assumption that one can replace the lower limit 0 by say \( \tau \) such that \( t \gg t - \tau \gg T_L \), so that during the interval \( \tau \leq s \leq t, v_{p_i}(x, 0 | s) \) is stationary, one arrives at the classic result that

\[
\frac{1}{2} \left[ \frac{d}{dt} \left< X_{p_i}(x, 0 | t)^2 \right> \right]_{t \to \infty} = \int_0^\infty R_{ij}(s) ds
\]

(12)

a result which is self consistent with a Gaussian or gradient diffusion process with a diffusion coefficient given by the RHS of Eq.(12). Returning to the form for the diffusion coefficient defined in Eq.(12) that is the extension to non-Gaussian fields, we note that with the Taylor Gaussian assumption for \( t \to \infty \), we are left with the result that

\[
D_{ij} = \int_0^t ds_1 \left< v'_{p_i}(x, t | s) v'_{p_j}(x, t) \right>
\]

(13)

which since \( \left< v'_{p_i}(x, t | s) v'_{p_j}(x, t) \right> \) is dependent only on \( t - s \) we get the same result as in Eq.(12) if

\[
\left< v'_{p_i}(x, t | s) v'_{p_j}(x, t) \right> = \left< v'_{p_i}(x, 0 | s) v'_{p_j}(x, 0 | t) \right>
\]

(14)
If the flow is homogeneous and stationary then these correlations since they refer to the same particle measured at two different times, will be independent of labeling position and times. That is we could change the labeling time from \(t\) to \(0\) in the correlation on the RHS of Eq. (14) and retain the labeling position \(x\) without changing the result. So the relationship in Eq. (14) is valid. The relevance of this independence on labelling times and positions is even more revealing when we consider the general result for the rate of mean square displacement given in Eq. (11) for all \(t\) and compare it with the form derived from the continuity equation

\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \cdot \langle \rho \mathbf{v}_p \rangle \tag{15}
\]

on the form for \(D_{ij}\) in Eq. (8) appropriate for non-Gaussian fields. That is if we release particles at time \(0\) and measure the dispersion at time \(t\) then the form of \(D_{ij}\) would imply that

\[
\langle \mathbf{v}_p(x, 0 | t), t \rangle X_{p}(x, 0 | t) \rangle = \langle \mathbf{v}_p(x, t), X_{p}(x, t | 0) \rangle - \int_0^t ds_1 \int_0^t ds_2 \left\langle \nabla \cdot \mathbf{v}_p(s_1), \mathbf{v}_p'(s_2), \mathbf{v}_p'(t) \right\rangle + \ldots
\]

The statistics associated with the correlation on the LHS of this equation is different from that determining the first term on the RHS of the equation: in LHS case, we have statistics derived from two Lagrangian variables where arguments for stationarity can only be invoked when \(t \to \infty\), whilst the case of the RHS is derived from a Lagrangian and an Eulerian variable. The two are only equal when \(t \to \infty\) or at small times \(t \ll T_L\) when the second term on the RHS is \(O(t/T_L)\) smaller. The term on the RHS is clearly a measure of the difference in the two sorts of statistics.

### 3. PDF FORMULATION

This represents an extension of previous work by this author (Reeks 1991, 1992) and several others (Zaichik 1991, Swailes 1997, Hyland et al. 1999, Pozorski & Minier 1999 and Simonin et al. 1999) in using an equation for the particle phase space probability to formally derive the two-fluid continuum equations for the particle phase.

#### 2.1 Definition and prescription of particle velocity field and its divergence

Using Stokes drag as an example, the particle equation of motion can be written as

\[
\frac{d\mathbf{v}}{dt} = \beta \{\mathbf{u}(x, t) - \mathbf{v}\} + \mathbf{g} \quad : \quad \frac{d\mathbf{x}}{dt} = \mathbf{v} \tag{16}
\]

where as before \(\mathbf{u}(x_p, t)\) is the underlying carrier flow velocity at position \(x\) at time \(t\). The solution can be written in several ways. First solving the set as a time problem,

\[
\mathbf{v} = \mathbf{V}_p(\omega, y, t | t) \quad ; \quad \mathbf{x} = \mathbf{X}_p(\omega, y, t' | t) \tag{17}
\]

i.e. the solution is the particle velocity/position at time \(t\), for a particle with initial velocity \(\omega\) and position \(y\) at time \(t'\), allowing for the possibility of \(t'\) being in the past or the future in relation to \(t\). Clearly these functions define the inverse relations

\[
\omega = \mathbf{V}_p(\mathbf{v}, x, t | t') \quad ; \quad y = \mathbf{X}_p(\mathbf{v}, x, t | t') \tag{18}
\]

So using these equations we could eliminate \(y\) from Eq. (17) and write an alternative solution, namely

\[
\mathbf{v} = \mathbf{v}_p(\omega, x, t' | t) \tag{19}
\]
That is the particle velocity at position \( \mathbf{x} \) at time \( t \) given that the particle velocity started out at time \( t' \) with a velocity \( \omega \). \( \mathbf{v}_p(\omega, \mathbf{x}, t' \mid t) \) is the particle velocity field (in the context of the passive scalar dispersion in Section 2), which satisfies the equation

\[
\frac{d\mathbf{X}_p}{dt} = \mathbf{v}_p(\omega, \mathbf{X}_p, t' \mid t). \tag{20}
\]

So we have

\[
\frac{d}{dt} \left\{ \frac{\partial \mathbf{X}_p(\omega, \mathbf{y}, t' \mid t)}{\partial y_j} \right\} = \left( \frac{\partial \mathbf{v}_p}{\partial \mathbf{X}_p} \right) \left( \frac{\partial \mathbf{X}_p}{\partial y_j} \right). \tag{21}
\]

Given that the initial conditions imply that

\[
\frac{\partial \mathbf{X}_p}{\partial y_j} = \delta_{ij} \text{ at } t = t', \tag{22}
\]

then we would have directly from Eq.(21) that

\[
J = \left| \frac{\partial \mathbf{X}_p(\omega, \mathbf{y}, t' \mid t)}{\partial \mathbf{y}} \right| = \exp \left\{ \int_{t'}^t ds \, \nabla \cdot \mathbf{v}_p(\omega, \mathbf{y}, s) \right\} |_{\mathbf{y} = \mathbf{X}_p(\mathbf{x}, t,s)} \tag{23}
\]

### 2.2 Closure of the PDF Equation

If \( W(\mathbf{x}, \mathbf{v}, t) \) is the phase space density for a particle with velocity \( \mathbf{v} \) and position \( \mathbf{x} \) at time \( t \) subject to the equation of motion defined in Eq.(16) for one realisation of the carrier flow filed \( \mathbf{u}(\mathbf{x}, t) \), then the equation for \( \langle W(\mathbf{v}, \mathbf{x}, t) \rangle \) the PDF for a particle to have \( (\mathbf{v}, \mathbf{x}, t) \) is obtained by averaging the Liouville equation thus,

\[
\left[ \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot \beta \{ \langle \mathbf{u}(\mathbf{x}, t) \rangle - \mathbf{v} \} \right] \langle W \rangle = -\frac{\partial}{\partial \mathbf{v}} \cdot \beta \langle \mathbf{u}'(\mathbf{x}, t) W \rangle \tag{24}
\]

where \( \langle \mathbf{u}(\mathbf{x}, t) \rangle \) and \( \mathbf{u}'(\mathbf{x}, t) \) are the mean and fluctuating components of \( \mathbf{u}(\mathbf{x}, t) \). We require therefore a closed expression for \( \langle \mathbf{u}'(\mathbf{x}, t) W \rangle \). In reality we consider a closed
expression for the specific case when $W$ is a response function $G$, that is it is the solution for an instantaneous point source $\delta(v - v')\delta(x - x')\delta(t - t')$. Thus $\langle G \rangle$ is the solution of the PDF equation Eq.(24) with the instantaneous point source added to the RHS of the equation. Knowing $\langle G \rangle$ we have for $\langle W(v,x,t) \rangle$

$$\langle W(v,x,t) \rangle = \int dv' dx' \langle G(v,x,t|v',x',t') \rangle \rho(v',x',t') dv' dx'$$

(25)

where $\rho(v',x',t')$ is some initial distribution of $\langle W \rangle$ at time $t'$. With reference to Eqs.(17), we can write the solution for $\langle G \rangle$ formally as

$$\langle G \rangle = \langle \delta(v - V_p(v',x',t'|t))\delta(x - X_p(v',x',t'|t)) \rangle$$

(26)

However using the definition of the particle velocity field $v_p(v',t'|x,t)$ we can write this alternatively as

$$\langle G \rangle = \langle \delta(v - V_p(v',t'|x,t))\delta(x - \int_{t'}^t ds v_p(v',t'|y,s) - x') \rangle \exp\{-\int_{t'}^t ds \nabla \cdot v_p(v',t'|y,s) \big|_{y=X_p(x,t|s)} \}$$

(27)

Similarly we can write down formally an expression for $\langle Gu \rangle$. This expression together with that for $\langle G \rangle$ are in form that we can process in a similar manner to the evaluation of $\langle \rho v_p \rangle$ for the passive scalar case: the only difference here is we are considering a process $[v_p(s), \nabla \cdot v_p(s), u(s); t' \leq s \leq t]$ as opposed to $[v_p(s), \nabla \cdot v_p(s); t' \leq s \leq t]$. We show in Appendix B that if this process is Gaussian, then $\beta \langle Gu \rangle$ is given exactly by

$$\beta \langle u(x,t)G(v,x,t|v',x',t') \rangle = - \left( \mu \cdot \frac{\partial}{\partial v} + \Delta \cdot \frac{\partial}{\partial x} \right) \langle G \rangle + \gamma \langle G \rangle$$

(28)

where

$$\mu = \beta \langle u'(x,t)v_p(t) \rangle$$

$$\Delta = \beta \langle u'(x,t)x_p(t) \rangle$$

$$\gamma = -\beta \int_{t'}^t ds \langle u'(x,t)\nabla \cdot v_p(s) \rangle ,$$

(29)

where

$$v_p(s) \equiv v_p(v',t'|x_p(x,t|s),s) \quad \nabla \cdot v_p(s) \equiv \nabla \cdot v_p(v',t'|y,s) \big|_{y=x_p(x,t|s)}$$

$$x_p(t) \equiv X_p(x,t|0) = \int_0^t v_p(v',t'|x_p(x,t,s),s) ds$$

(30)

The form of the net force per unit mass of particles due to the turbulence given in Eq.(28) is therefore composed of two parts: a *diffusive force* (gradient of a stress tensor) which depend upon gradients in the particle velocity and position [the bracketed term on the RHS of Eq.(28)] and a *body force* which depends upon the local compressibility of instantaneous particle velocity field along a particle trajectory [the second term in Eq.(28)]. The general form of this *turbulent force* has been obtained before by several authors (Reeks 1992, Swailes et. al. 1997, Pozorski and Minier 1999, Hyland et. al. 1999) but the precise form for the body force is different from the one derived here and leads to
the so-called problem of spurious drift; that is there is a drift term that persists in cases where the particles follow the underlying incompressible flow ($\beta^{-1} \rightarrow 0$) so that where at equilibrium the particles ought to be fully mixed with the flow, the existence of the spurious drift leads to a build up of concentration in regions of low turbulence intensity. It is a feature that is common in certain types of simple random walk simulation of particle dispersion in inhomogeneous turbulence (where the underlying flow field is essentially 1-D and cannot of its own accord satisfy continuity of flow if it is spatially varying. The form derived here does not suffer from this serious defect, the drift velocity $v_d$ in this case $\beta^{-1} \gamma$, clearly vanishes when the particle follow the flow, because $\nabla \cdot \mathbf{v}_p(s)$ is the same as that of the underlying carrier flow which is necessarily zero.

As an illustration of the influence of turbulent structures I have considered the dispersion of particles in a random flow field which consists of pairs of counter-rotating vortices (see Fig.1) with randomly generated vorticity that shifts randomly in position as the timescale of the vorticity changes randomly from one value to the next in time. In the case of a flow field in which the location and periodicity of the structures is fixed, particles accumulate at the stagnation points. That is the process is equivalent to diffusion plus a drift directed towards the stagnation point. As an example Fig.2 shows the difference in behaviour between a 1 D flow field in which the particles are constrained to move only in the x-direction and when they allowed to move in the y -direction (fully 2D vortex flow field). The difference illustrates the difference between spurious drift (arising from a 1 D carrier flow field which is compressible) and the case of an incompressible 2D carrier flow.

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APPENDIX A

A1. Gaussian Process

We expand $\rho \left( \mathbf{r} - \int_{0}^{t} \mathbf{v}_{p}(s)ds, 0 \right)$ in Eq.(4) as a Taylor’s series about $\rho(\mathbf{r}, 0)$ so that formally

$$
\rho(\mathbf{r}, t) = exp \left\{ - \left[ \int_{0}^{t} \nabla \cdot \mathbf{v}_{p}(s)ds + \int_{0}^{t} ds \mathbf{v}_{p}(s) \cdot \frac{\partial}{\partial \mathbf{r}} \right] \right\} \rho(\mathbf{r}, 0).
$$

(32)

We now suppose that both $\mathbf{v}_{p}(s)$ and $\nabla \cdot \mathbf{v}_{p}(s)$ to be a continuous processes whose statistics are correlated. That is $\mathbf{v}_{p}(s)$ is the limit of the discrete process

$$
[\mathbf{v}_{p}(s)] = N_{\to \infty} [\mathbf{v}_{p}(s_{1}), \mathbf{v}_{p}(s_{1})...\mathbf{v}_{p}(s_{j})...\mathbf{v}_{p}(s_{N})]$$

$$
j_{\tau} = s \tau \text{ with } N_{\tau} = s.
$$

(33)

Similarly for $\nabla \cdot \mathbf{v}_{p}(s)$. For convenience we specify a vector $\mathbf{q}(s)$

$$
\mathbf{q}(s) = [\mathbf{v}_{p1}(s), \mathbf{v}_{p2}(s), \mathbf{v}_{p3}(s), \nabla \cdot \mathbf{v}_{p}(s)]
$$

(34)

whose statistics we specify through the characteristic functional $M[\phi(s)]$ given formally by

$$
M[\phi(s)] = \left\langle exp \left( i \int_{0}^{t} \phi(s) \cdot \mathbf{q}(s)ds \right) \right\rangle
$$

where $\phi(s)$ is an arbitrary vector function of time

(35)
and we further assume that \( q(s) \) is Gaussian so that

\[
M[\phi(s)] = \exp \left\{ i \int_0^t \langle q(s) \rangle \cdot \phi(s) ds \right. \\
\left. - \frac{1}{2} \int_0^t ds_1 \int_0^t ds_2 \langle q'_i(s_1)q'_j(s_2) \rangle \phi_i(s_1)\phi_j(s_2) \right\} 
\]  
(36)

where

\[
\{\langle q_i(s) \rangle = W_i; q'_i(s_1) = q_i(s_1) - W_i\} \quad i \leq 3; \quad \{\langle q_i(s) \rangle = 0; q'_i(s) = q_i(s)\} \quad i = 4
\]

We recognize from the definition of the characteristic functional that

\[
\langle \rho(r, t) \rangle = M[i\phi(t)] \rho(r, 0)
\]

with \( \phi_i(t) = \frac{\partial}{\partial x_i} \) for \( i \leq 3 \)

\[
= 1 \quad i = 4
\]  
(37)

and

\[
\langle v_{pi}(t)\rho(r, t) \rangle = -\frac{\delta M[i\phi(s)]}{\delta \phi_i(t)} \rho(r, 0) \text{ for } i \leq 3
\]  
(38)

Substituting the Gaussian functional for \( M \) given in Eq.(36) into Eq.(38) and performing the functional differentiation we obtain

\[
\langle v_{pk}(t)\rho(r, t) \rangle = \left\{ \langle q_k(t) \rangle + i \int_0^t \langle q_4(s)q_k(t) \rangle \phi_4(s) ds + i \sum_{i=1}^3 \int_0^t ds \langle q_i(s)q_k(t) \rangle \phi_i(s) \right\} \langle \rho(r, t) \rangle
\]  
(39)

Substituting the values for \( \phi_i(s) \) in Eq.(37) into Eq.(39) we obtain finally

\[
\langle v_{pk}(t)\rho(r, t) \rangle = \left\{ \langle v_{pk}(r, t) \rangle - \int_0^t \langle v_{pk}(t) \nabla \cdot v_{pk}(s) \rangle ds \right\} \langle \rho(r, t) \rangle
\]

\[
- \int_0^t ds \left\langle v'_{pk}(t)v'_{pi}(s) \right\rangle \frac{\partial}{\partial x_i} \langle \rho(r, t) \rangle
\]  
(40)

\[\text{A1. Non-Gaussian Process}\]

The same analysis can be extended to consider dispersion and drift in which \( v_{p}(s) \) and \( \nabla \cdot v_{p}(s) \) are jointly non-Gaussian in which we express the characteristic functional \( M[\phi(t)] \) in terms of the cumulants of \( q(t) \), i.e.

\[
M[\phi(s)] = \exp \left( \int_0^t \langle q(s) \rangle \cdot \phi(s) ds + \sum_{m=2}^{\infty} \sum_{1 \leq \alpha_1 \leq \ldots \leq \alpha_m \leq n} \frac{\alpha_1! \alpha_2! \ldots \alpha_m!}{m!} \int_0^s ds_1 \int_0^{s_1} ds_2 \ldots \int_0^{s_{m-1}} ds_m \times \right.
\]

\[
\left. \times \langle q'_{\alpha_1}(s_1)q'_{\alpha_2}(s_2) \ldots q'_{\alpha_m}(s_m) \rangle \times \right. \nonumber
\]

\[
\times \phi_{\alpha_1}(s_1)\phi_{\alpha_2}(s_2) \ldots \phi_{\alpha_m}(s_m) \right) \nonumber
\]  
(41)

where \( \|\langle q'_{\alpha_1}(s_1)q'_{\alpha_2}(s_2) \ldots q'_{\alpha_m}(s_m) \rangle\| \) represent the cumulants of \( q(t) \). Using this form for \( M[\phi(s)] \) and Eq.(38) we obtain:

\[
\langle v_{pk}(t)\rho(r, t) \rangle = \langle \rho(r, t) \rangle W_k + \sum_{m=1}^{\infty} \left( \frac{(-1)^m}{m!} \int_0^t ds_1 \ldots \int_0^{s_{m-1}} ds_m \times \right.
\]

\[
\left. \times \langle q'_{\alpha_1}(s_1)q'_{\alpha_2}(s_2) \ldots q'_{\alpha_m}(s_m) \rangle \times \right. \nonumber
\]

\[
\times \phi_{\alpha_1}(s_1)\phi_{\alpha_2}(s_2) \ldots \phi_{\alpha_m}(s_m) \right) \nonumber
\]  
(42)

\[\text{where}\]
with \( \phi(t) \) given by Eqs.\([37]\). So picking out the contribution to the drift and to the gradient diffusion from the correlation of the process \([v_p(s)]\) with the process \([\nabla \cdot v_p(s)]\) we can write Eqs.\([42]\) more transparently as

\[
\langle v_{pk}(t)\rho(r, t) \rangle = \left\{ W_k - \sum_{m=1}^{\infty} \left( \frac{(-1)^{m+1}}{m!} \int_0^t ds_1 \ldots \int_0^t ds_m \times \right) \right. \\
\left. \left\| \langle \nabla \cdot v_{p(s_1)} \ldots \nabla \cdot v_{p(s_m)} \rangle v_{pk}'(t) \right\| \right\} \langle \rho(r, t) \rangle
\]  

(43)

So to first order in the triple moments of \([q(t)]\) the convective velocity \(v_d\) and Diffusion coefficients \(D_{ij}\) are respectively

\[
v_d = \langle v_p(r, t) \rangle - \int_0^t ds_1 \langle \nabla \cdot v_p(s_1) v_{p}'(t) \rangle + \frac{1}{2} \int_0^t ds_1 \int_0^t ds_2 \langle \nabla \cdot v_p(s_1) \nabla \cdot v_p(s_2) v_{p}'(t) \rangle + \ldots
\]

(45)

\[
D_{ij} = \int_0^t ds_1 \langle v_{pi}'(s_1) v_{pj}'(t) \rangle - \int_0^t ds_1 \int_0^t ds_2 \langle \nabla \cdot v_p(s_1) \nabla \cdot v_p(s_2) v_{pj}'(t) \rangle
\]

(46)

So the diffusion coefficient is derived from two parts: one which is appropriate for incompressible flows if the process and the other which is appropriate for compressible flows for non-Gaussian processes.

APPENDIX B Evaluation of \(\langle Gu(x, t)\rangle\)

We can formally write Eq.\([27]\) as

\[
\langle G \rangle = \left\langle \exp \left\{ - \left[ v_p'(t) \cdot \frac{\partial}{\partial x} + \int_{t'}^t ds v_p'(s) \cdot \frac{\partial}{\partial x} + \int_{t'}^t ds \nabla \cdot v_p(s) \right] \right\} \right\rangle G^{(0)}(v, x, t|v', x', t')
\]

(47)

where \(v_p(s)\) is used as shorthand for \(v_p(v', t|X_p(x, t|s), s)\) and a similar short hand of \(\nabla \cdot v_p(s)\) for \(\nabla \cdot v_p(v', t|X_p(x, t|s), s)\). and \(v_p(s)\) is the fluctuating value of \(v_p(s)\) with respect to its average value \(\langle v_p(s) \rangle\). \(G^{(0)}(v, x, t)\) is the response function

\[
G^{(0)} = \delta(v - \langle v_p(t) \rangle) \delta(x - \int_{t'}^t ds (\langle v_p(s) \rangle - x'))
\]

(48)

So as for the passive scalar case we consider the statistical process

\[
q(s) = [v_{p1}'(s), v_{p2}'(s), v_{p3}'(s), u_1'(s), u_2'(s), u_3'(s), \nabla \cdot v_p(s)]
\]

(49)

with a given characteristic functional \(M[\phi(s)]\) which we will assume is a Gaussian functional. We have thus as before

\[
\langle G \rangle = M[i\phi(s)]
\]

(50)

with \(\phi_i(s) = \delta(s-t) \frac{\partial}{\partial x_i} + \frac{\partial}{\partial x_i} \) for \(1 \leq i \leq 3\)

\[
= 0 \quad \text{for} \quad 4 \leq i \leq 6
\]

\[
= 1 \quad \text{for} \quad i = 7
\]

(51)
and
\[
\langle u_i(t)G \rangle = \frac{\delta M[\phi_{i+3}(s)]}{\delta \phi_{i+3}(t)} G^{(0)}(v, x, t|v', x', t)
\]  

(52)

Performing this functional differentiation on the Gaussian Characteristic functional, leads to the closed expression

\[
\langle u'_i(t)G \rangle = -\left\{ \langle u'_i(t)v'_j(t) \rangle \frac{\partial}{\partial v_j} + \int_t^t ds \langle u'_i(t)v'_j(s) \rangle \frac{\partial}{\partial x_j} + \int_t^t ds \langle u'_i(t) \nabla \cdot v_p(s) \rangle \right\} \langle G \rangle
\]

(53)