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On model equations for particle dispersion in inhomogeneous turbulence

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Abstract

Comparisons are made between the Advection–Diffusion Equation (ADE) approach for particle transport and the two-fluid model approach based on the PDF method. In principle, the ADE approach offers a much simpler way of calculating the inertial deposition of particles in a turbulent boundary layer than that based on the PDF approach. However the ADE equations that have recently been used are only strictly valid for a simple Gaussian process when particle inertia is small. Using a prescribed, but in general non-Gaussian random particle velocity field, it is shown that the net particle mass flux contains a drift term in addition to that from the mean velocity of the particle velocity field, associated with the compressibility of the velocity field. Furthermore the diffusive flux in general depends not only upon the gradient of the mean concentration (true only for a Gaussian random flow field) but also upon higher order derivatives whose relative contribution depends on diffusion coefficients $D_{ijk\dots}$ etc. These coefficients depend upon the statistical moments associated with random displacements and compressibility of the particle flow field along particle trajectories which in turn depend upon particle inertia. In contrast the PDF approach offers the advantage of using a simple gradient (Gaussian) approximation in particle phase space which can lead to a non-Gaussian spatial dispersion process when particle inertia is important. Conditions based on the particle mean free path are derived for which a simple ADE is appropriate. Some of the features of particle transport in an inhomogeneous turbulent flow are illustrated by examining particle dispersion in a random flow field composed of pairs of counter rotating vortices which has an rms velocity which increase linearly from a stagnation point.

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1. Introduction

This paper is about ways of modelling the transport of particles in inhomogeneous turbulence. The practical example and most challenging, is that of particle deposition in a fully developed turbulent boundary layer for which there are numerous ad hoc models (see e.g. the review by Papavergos and Hedley, 1984 and more recently Young and Leeming, 1997). However, more generally, there are two basic approaches which have been used: the so-called *Lagrangian tracking* approach where individual particles are tracked through a random flow field typical of the turbulence by solving the individual particle equation of motion; and an *Eulerian two-fluid* approach where the dispersed particle phase is treated as a fluid in much the same way as the carrier phase, namely by a set of continuum equations which represent the conservation of mass, momentum and energy within some elemental volume of the dispersed phase. This paper is devoted to the latter of these two approaches.

Whilst in principle the so-called traditional two-fluid approach is computationally very efficient to apply, the draw-back is that until fairly recently, the constitutive relations/closure approximations necessary for the solutions of the continuum equations have been heuristic/empirical and not directly traceable to the underlying particle equations of motion. Furthermore the boundary conditions necessary for uniqueness, are not compatible with the natural boundary conditions of the system. Very recently, Young and Leeming (YL) (1997) dramatically reduced the complexity of these model equations by using a simple advection diffusion equation (ADE) where the advection is provided by the underlying particle velocity field. So the problem of particle dispersion and deposition is reduced to one of passive scalar diffusion in a compressible particle velocity field whose statistics are not prescribed (as in traditional passive scalar diffusion) but calculated from the particle equation of motion. Unlike the two-fluid approach where the continuum equations are coupled, the ADE is separated from the equation for the mean particle velocity field which is used as an input to the ADE itself. However the transport equation for the mean velocity and the form of the particle diffusion coefficient were subject to certain assumptions which were heuristic in nature and not rigorously derived. That being said, in the case of particle deposition in a turbulent boundary layer, the model successfully reproduced the main deposition features from a single set of equations without the use of any adjustable constants.

In recent years, significant progress has been made in modelling dispersed flows with the development of a Probability Density Function (PDF) approach which is similar to the Kinetic Theory of gases in the sense that the continuum equations for the dispersed phase and their constitutive relations are derived from a master equation which represents the transport of particles in phase space. In the more traditional Kinetic Method (KM) inspired by the early work of Buyevich (1971, 1972a,b), the PDF is associated with the particle velocity and position. In the more recent approach due to Simonin et al. (1993), the PDF is associated with particle velocity, position and the carrier flow velocity encountered by the particle. Closure approximations are made in particle phase space rather than in configuration space which in turn yields a set of constitutive relations for the mass, momentum and energy equations for the dispersed phase. These closure approximations are legitimate in the sense that they are formally related to the underlying equations of motion and preserve realizability. The two-fluid model equations derived in this way, have thus a much sounder theoretical basis, the only constants involved being those of the particle equations of motion and statistics of the carrier flow itself.

The purpose of this paper is to make some comparisons of the ADE models of Young and Leeming (YL) (1997) and also more recently Cerbelli et al. (2001) for predicting particle deposition in turbulent pipe flow with the set of continuum equations based on the PDF approach (Reeks, 2001). In particular certain ad hoc assumptions about the closure of the averaged equations in the YL and the CGS models need to be examined in the light of more formal closure approximations based on the PDF method (Reeks, 2001). The purpose is to show whether and if so to what order in the particle response time these ad hoc closure models are valid. The PDF and two-fluid approaches use methods and equations based on density weighted averages whilst the advection diffusion equations (ADEs) involve direct ensemble averaged quantities used. What therefore are the advantages and disadvantages of either approach?

In Section 2 the YL and CGS models are reviewed. In Section 3, I then examine some of the assumptions and approximations that were made in these models by considering passive scalar dispersion of particles in a compressible flow field whose statistics are prescribed along a particle trajectory—this includes not only the particle velocity and position at time t but also the statistics of the compressibility of the particle flow field. This allows a precise definition of the particle diffusion coefficient and advection velocity. In Section 4, I present the two-fluid model equations for the dispersed phase based on the KM formulation of the PDF approach which are subsequently compared with the ADE approach in Section 5. Then finally in Section 6, some of the basic features of the ADE and PDF approaches are illustrated quantitatively for particle transport in a simple inhomogeneous turbulent flow where the carrier flow mean square velocity varies linearly with the distance from a fixed stagnation point.

2. Advection–diffusion models

The YL model starts from the continuity equations of the dispersed particle phase, namely

$$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot \mathbf{v}\rho = 0 \tag{2.1}$$

where $\rho(\mathbf{x}, t)$ is the instantaneous particle mass density at position $\mathbf{x}$ at time t transported by a velocity field $\mathbf{v}(\mathbf{x}, t)$. The concentration and velocity fields are separated into mean ensemble averages and fluctuating components. Thus,

$$\rho(\mathbf{x}, t) = \langle \rho(\mathbf{x}, t) \rangle + \rho'(\mathbf{x}, t) \tag{2.2}$$

$$\mathbf{v}(\mathbf{x}, t) = \langle \mathbf{v}(\mathbf{x}, t) \rangle + \mathbf{v}'(\mathbf{x}, t) \tag{2.3}$$

where $\langle \ldots \rangle$ means an ensemble average. So taking the ensemble average of the continuity equation, Eq. (2.1) gives:

$$\frac{\partial}{\partial t}\langle \rho \rangle + \underline{\nabla} \cdot \mathbf{J} = 0 \tag{2.4}$$

where the mass flux $\mathbf{J}$ is given by

$$\mathbf{J} = \langle \mathbf{v} \rangle \langle \rho \rangle + \langle \mathbf{v}' \rho' \rangle \tag{2.5}$$

YL refer to the first term as a convection term (in the sense that the convection velocity $\langle \mathbf{v} \rangle$ is independent of particle concentration), and the second part as a diffusive term, that is, it depends upon the gradients of the mean particle concentration. In particular they assume that this term can be represented to a good approximation by a gradient approximation of the form

$$\langle \mathbf{v}' \rho' \rangle = -(D_{\mathrm{B}} + D_{\mathrm{turb}}) \underline{\nabla} \langle \rho \rangle \tag{2.6}$$

where D_{B} is the Brownian diffusion coefficient and D_{turb} the turbulent diffusion coefficient of the particle. YL set D_{turb} to be the same as that of the local fluid element dispersion coefficient. The equation for $\mathbf{v}(\mathbf{x}, t)$ is

$$\frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} = \frac{\Phi_{\mathrm{D}}}{\tau_{\mathrm{p}}} (\mathbf{u} - \mathbf{v}) + \mathbf{F}_{\mathrm{L}} + \mathbf{g} \tag{2.7}$$

where:

- $\mathrm{D}/\mathrm{D}t$ is the rate of change with respect to time along an individual particle trajectory;
- the first term on the RHS is the drag force (per unit mass of particle) acting on an individual particle with Stokes relaxation time τ_{p}, moving with the velocity $\mathbf{v}(\mathbf{x}, t)$ at $\mathbf{x}, t$ where the *local* gas carrier flow velocity is $\mathbf{u}(\mathbf{x}, t)$; Φ_{D} is a factor representing the departure from Stokes drag and is a function of the particle Reynolds number;
- $\mathbf{F}_{\mathrm{L}}$ is the particle lift force (per unit mass): in the YL model the form due to Saffman is adopted, assuming that the major source of lift arises from the local mean shear and the relative velocity between particle and carrier flow in the axial direction;
- $\mathbf{g}$ is the acceleration due to gravity.

We shall refer to this ADE model as an advection with simple gradient diffusion model or a simple ADE model for short.

A transport equation for the mean velocity $\langle \mathbf{v} \rangle$ is found by ensemble/Reynolds averaging Eq. (2.7), namely

$$\frac{\mathrm{D}\langle \mathbf{v} \rangle}{\mathrm{D}t} = -\langle (\mathbf{v}' \cdot \underline{\nabla}) \mathbf{v}' \rangle + \frac{\Phi_{\mathrm{D}}}{\tau_{\mathrm{p}}} (\langle \mathbf{u} \rangle - \langle \mathbf{v} \rangle) + \langle \mathbf{F}_{\mathrm{L}} \rangle + \mathbf{g} \tag{2.8}$$

where $\mathrm{D}/\mathrm{D}t$ now refers to $\partial/\partial t + \langle \mathbf{v} \rangle \cdot \underline{\nabla}$, i.e. the rate of change for transport by $\langle \mathbf{v} \rangle$. In both the YL and CGS models it is assumed that the particle velocity field $\mathbf{v}(\mathbf{x}, t)$ is fully developed i.e. the statistical moments of $\mathbf{v}(\mathbf{x}, t)$ are all independent of time and $\mathrm{D}/\mathrm{D}t = \langle \mathbf{v} \rangle \cdot \underline{\nabla}$. Using the continuity equation Eq. (2.1), YL write the first term on the RHS side in terms of the particle velocity covariance, namely

$$\langle (\mathbf{v}' \cdot \underline{\nabla}) \mathbf{v}' \rangle = \langle \underline{\nabla} \cdot \mathbf{v}' \mathbf{v}' \rangle - \langle \mathbf{v}' \underline{\nabla} \cdot \mathbf{v}' \rangle \approx \langle \underline{\nabla} \cdot \mathbf{v}' \mathbf{v}' \rangle - \langle \mathbf{v}' \mathbf{v} \cdot \underline{\nabla} \ln \rho \rangle \tag{2.9}$$

so that the transport equation for $\langle \mathbf{v} \rangle$ is given as

$$\frac{\mathrm{D}\langle \mathbf{v} \rangle}{\mathrm{D}t} \approx -\langle \underline{\nabla} \cdot \mathbf{v}' \mathbf{v}' \rangle + \frac{\overline{\Phi}_{\mathrm{D}}}{\tau_{\mathrm{p}}} (\langle \mathbf{u} \rangle - \langle \mathbf{v} \rangle) + \langle \mathbf{F}_{\mathrm{L}} \rangle + \mathbf{g} + \langle \mathbf{v}' \mathbf{v} \cdot \underline{\nabla} \ln \rho \rangle \tag{2.10}$$

where $\overline{\Phi}_{\mathrm{D}}$ refers to the drag factor as a function of the average particle Reynolds number.

YL argue that the contribution from the last term in Eq. (2.10) is small compared to that from the other terms because large gradients in concentration are unlikely to occur with large convection velocities. So ignoring this term and gravity, the transport equation for the steady state mean particle velocity field in the y-direction normal to the wall in turbulent pipe flow used by YL is given by

$$\langle v_y \rangle \frac{\partial \langle v_y \rangle}{\partial y} = -\frac{\partial \langle v_y'^2 \rangle}{\partial y} - \frac{\overline{\Phi}_{\mathrm{D}}}{\tau_{\mathrm{p}}} \langle v_y \rangle + \langle F_y \rangle \tag{2.11}$$

This together with the gradient diffusion Eq. (2.6) are the basic equations used by YL for deposition in turbulent pipe flow. YL recognize the first term on the RHS of Eq. (2.11) as the origin of the turbophoretic velocity referred to previously (Reeks, 1983) and replace the particle mean square velocity in this term it by the form appropriate for local homogeneity, namely

$$\langle v_y'^2 \rangle = \Gamma(\tau_{\mathrm{p}}/\tau_{\mathrm{g}}) \langle u_y'^2 \rangle \tag{2.12}$$

where $\langle u_y'^2 \rangle$ is the local gas flow mean square velocity normal to the wall and the ratio Γ is based on an exponential decay for the Lagrangian velocity autocorrelation of the local carrier gas flow with integral time scale τ_{g}, namely

$$\Gamma = \frac{\tau_{\mathrm{g}}}{\tau_{\mathrm{p}} + \tau_{\mathrm{g}}} \tag{2.13}$$

CGS adopt a similar ADE approach to YL but retain the last term involving the compressibility in Eq. (2.10), approximating it by

$$\langle \mathbf{v}'\mathbf{v} \cdot \underline{\nabla} \ln \rho \rangle \approx \langle \mathbf{v}'\mathbf{v}' \rangle \cdot \underline{\nabla} \ln \langle \rho \rangle \tag{2.14}$$

The inclusion of this term gave better agreement with their corresponding DNS measurements of deposition than those based on the YL model.

3. Closure approximations for advection–diffusion

I have recently considered the problem of advection/diffusion of particles in a random compressible velocity field (Reeks, 2001). The situation is precisely the same as the case of particles transported in an incompressible carrier flow field. That is, we know that because the carrier flow field contains structures like vortices and straining regions and the way particles interact with those structures, it will demix a suspension of particles, segregating the particles into regions of high strain rate. Alternatively, we can argue equivalently that in the process of segregation, a particle velocity flow field is produced which is spatially random and compressible and hence the demixing. So the analysis of particle dispersion is similar to that of a passive scalar in an incompressible velocity field except that in addition to the statistics of the particle velocity along a particle trajectory we also prescribe the compressibility $\underline{\nabla} \cdot \mathbf{v}$ along a particle trajectory. In particular an advection-diffusion process was considered for which the statistical process for particle displacements in position and compressibility are prescribed about a given point $\mathbf{x}, t$. Let this process be denoted by $[\underline{\Delta}\mathbf{x}(\mathbf{x}, t|s), \underline{\nabla} \cdot \mathbf{v}(\mathbf{x}, t|s)]$ where $\mathbf{x}, t|s$ denotes a particle starting out somewhere in the flow continuum at time s and arriving at $\mathbf{x}$ at time t., i.e. we are concerned with all trajectories that pass through $(\mathbf{x}, t)$ (the trajectories that may start off from some initial set of conditions will necessarily be a subset of all those trajectories). If this process is jointly Gaussian, it was shown that the net mass flux is precisely given by:

$$\begin{aligned}\langle \mathbf{v}(\mathbf{x},t)\rho(\mathbf{x},t)\rangle = &\left\{\langle \mathbf{v}(\mathbf{x},t)\rangle - \int_0^t \langle \mathbf{v}'(\mathbf{x},t)\nabla\cdot\mathbf{v}(\mathbf{x},t|s)\rangle\,\mathrm{d}s\right\}\langle\rho(\mathbf{x},t)\rangle \\ &- \left\langle \mathbf{v}'_{\mathrm{p}}(\mathbf{x},t)\underline{\Delta}\mathbf{x}(\mathbf{x},t|s)\right\rangle\cdot\underline{\nabla}\langle\rho(\mathbf{x},t)\rangle \end{aligned} \tag{3.15}$$

This flux differs from that for advection in an incompressible flow field in that the advection from the ensemble average of the instantaneous local convective velocity is augmented by a 'drift' velocity that depends upon the correlation of the log of the compression C (measured by the time integral of the compressibility along a particle trajectory) with the local fluctuating convective velocity. This contribution to the advective flux was first recognized by Maxey (1987) in the context of particles settling under gravity in isotropic, homogeneous and stationary turbulence. Without gravity in homogeneous turbulence, the contribution is necessarily zero, but in inhomogeneous flows as is the case of near wall turbulence, this is not the case, i.e. this term contributes to a drift velocity in general towards the wall arising not only because the particle flow velocity field is compressible but also inhomogeneous. As in the case of settling in homogeneous turbulence, it is relatively small for particles with both small and large inertia, with a maximum value somewhere in between, i.e. for an intermediate Stokes number $\sim$1. [1] The second term on the RHS of Eq. (3.15) is the diffusive flux for which the diffusion coefficients associated with particular axes have the same form as that due to Taylor for passive scalar dispersion in homogeneous stationary incompressible turbulence, except that the displacements here refer back in time to the starting time, whereas in Taylor's formula the displacements are forward in time from the starting time: strictly speaking then diffusion coefficients defined in Eq. (3.15) are backward diffusion coefficients and Taylor's formula represents forward diffusion coefficients (in homogeneous flows backward and forward defined diffusion coefficients are the same because of reversibility).

3.1. Result for non-Gaussian processes

If, in general, the statistics of the process $[\underline{\Delta}\mathbf{x}(\mathbf{x},t|s), \nabla\cdot\mathbf{v}(\mathbf{x},t|s)]$ are non-Gaussian, then it was shown (Reeks, 2001) that the particle mass current is compounded of a convective/drift term $\mathbf{v}_{\mathrm{d}}\langle\rho(\mathbf{x},t)\rangle$, where to first order in the triple moment of this process

$$\begin{aligned}\mathbf{v}_{\mathrm{d}} = &\langle \mathbf{v}(\mathbf{x},t)\rangle - \int_0^t \mathrm{d}s_1\langle\nabla\cdot\mathbf{v}(\mathbf{x},t|s_1)\mathbf{v}'(\mathbf{x},t)\rangle + \frac{1}{2}\int_0^t \mathrm{d}s_1 \\ &\times \int_0^t \mathrm{d}s_2\langle \mathbf{v}'(\mathbf{x},t)\nabla\cdot\mathbf{v}(\mathbf{x},t|s_1)\nabla\cdot\mathbf{v}(\mathbf{x},t|s_2)\rangle + \cdots \end{aligned} \tag{3.16}$$

and a dispersive flux $\mathbf{j}_{\mathrm{diff}}$ which is no longer simple gradient diffusion but depends as well upon higher order derivatives of the mean concentration, i.e.

[1] The Stokes number here is the Stokes relaxation time/typical timescale of the turbulent motion.

$$\mathbf{j}_{\text{diff}} = -\left(D_{ij}\frac{\partial}{\partial x_j} + D_{ijk}\frac{\partial^2}{\partial x_j\,\partial x_k} + \cdots\right)\langle\rho(\mathbf{x},t)\rangle \tag{3.17}$$

where the coefficients D_{ijk} etc. are dependent on increasing higher order moments of the process $[\Delta\mathbf{x}_i(\mathbf{x},t|0),\ v_j(\mathbf{x},t),\ \nabla\cdot\mathbf{v}_{\text{p}}(\mathbf{x},t|s)]$. In particular

$$D_{ij} = \int_0^t \mathrm{d}s_1\left\langle\Delta\mathbf{x}_i(\mathbf{x},t|0)v_j'(\mathbf{x},t)\right\rangle\cdots - \int_0^t \mathrm{d}s_1\langle\Delta\mathbf{x}_i(\mathbf{x},t|0)v_j(\mathbf{x},t)\nabla\cdot\mathbf{v}_{\text{p}}(\mathbf{x},t|s_1)\rangle + \tag{3.18}$$

4. Two-fluid models based on the PDF approach

In the traditional two-fluid approach, the *continuum* equations are obtained by averaging the instantaneous mass, momentum and energy equations of the particle phase over all realisations of the turbulent carrier flow field. Thus for a dilute inert non-reacting suspension of particles, all with the same mass and subject to Stokes drag as considered in the YL and CGS models,

$$0 = \frac{\partial\langle\rho\rangle}{\partial t} + \nabla\cdot(\langle\rho\rangle\bar{\mathbf{v}}) \tag{4.19}$$

$$\langle\rho\rangle\frac{\mathrm{D}\overline{v_i}}{\mathrm{D}t} = -\frac{\partial\langle\rho\rangle\overline{v_j'v_i'}}{\partial x_j} + \tau_{\text{p}}^{-1}(\langle u_i\rangle - \overline{v_i})\langle\rho\rangle + \tau_{\text{p}}^{-1}\langle\rho\rangle\overline{u_i'} \tag{4.20}$$

where most importantly the averages involved for the particle velocity are particle mass density weighted averages. [2] Thus in these equations $\overline{(..)}$ denotes a density weighted average of the quantity in brackets, so that:

$$\bar{\mathbf{v}} = \langle\rho\rangle^{-1}\langle\rho\mathbf{v}\rangle;\quad \mathbf{v}' = \mathbf{v} - \bar{\mathbf{v}};\quad \mathbf{u}' = \mathbf{u} - \langle\mathbf{u}\rangle \tag{4.21}$$

The density weighted carrier flow velocity on the RHS of the momentum equations has been referred to by Deutsch and Simonin (1991) as the flow velocity viewed by the particle. We note first that, unlike the ADE equations, the continuum equations are coupled equations and required closure or constitutive relations for the particle Reynolds stresses $-\langle\rho\rangle\overline{v_j'v_i'}$ and the carrier flow velocity viewed by the particle. The Reynolds stresses can be obtained via their transport equations (analogous to the transport equation for kinetic energy), derived in a similar manner to that for the net momentum equation (or via the PDF equation) using a closure approximation for the gradient of the Reynolds stress flux. The details are not important to this paper. A simple Boussinesq closure approximation for $\langle\rho\rangle\overline{u_i'}$ can be obtained from the PDF approach or more exactly via a transport equation (Simonin et al., 1993). The simple gradient approximation is the one we consider here because of its simplicity and because under certain conditions it lends itself to the interpretation of the momentum equation as an ADE equation. That is, the PDF approach gives for a process in which the displacements and compressibilities are jointly Gaussian:

[2] In this case number density and mass density would be the same because the particles are all assumed to have the same mass.

$$\langle\rho\rangle\overline{u_i'} = -\left\langle u_i'(\mathbf{x},t)\Delta\mathbf{x}_j(t)\right\rangle\frac{\partial\langle\rho\rangle}{\partial x_j} - \int_0^t \mathrm{d}s\left\langle u_i'(\mathbf{x},t)\nabla\cdot\mathbf{v}_\mathrm{p}(\mathbf{x},t\mid s)\right\rangle\langle\rho\rangle \tag{4.22}$$

If the process is non-Gaussian, then the diffusion coefficients and convection velocity are modified in a similar way to that indicated in Eqs. (3.16) and (3.18) for the particle mass flux. So the formula for this net mass flux is analogous to the net particle mass flux in the ADE approximation (3.15) and we might therefore legitimately refer to these diffusion coefficients as the fluid–particle diffusion coefficients. However the flux should be strictly be interpreted as a momentum flux, representing the net force per unit volume acting on the particles due to the turbulence. The properties of these diffusion coefficients in the case of a Gaussian process, have been discussed previously in uniform shearing and in homogeneous flow (Reeks, 1991, 1993).

4.1. The simple ADE as a special case of the momentum equations

Using this formula in Eq. (4.22), we can establish the circumstances under which the momentum equation would approximate to a simple ADE equation itself (i.e. simple gradient/Boussinesq diffusion and convection). So with this expression for $\langle\rho\rangle\overline{u_i'}$, we can rewrite the momentum equation as an equation for the net mass flux as

$$\overline{v_i}\langle\rho\rangle = \langle u_i\rangle\langle\rho\rangle - \epsilon_{ij}\frac{\partial\langle\rho\rangle}{\partial x_j} + v_{d_i}\langle\rho\rangle - \tau_\mathrm{p}\frac{\mathrm{D}\overline{v_i}}{\mathrm{D}t}\langle\rho\rangle \tag{4.23}$$

$$\epsilon_{ij} = \tau_\mathrm{p}\overline{v_i'v_j'} + \left\langle u_i'(\mathbf{x},t)\Delta\mathbf{x}_j(t)\right\rangle \tag{4.24}$$

$$v_{d_i} = -\int_0^t \mathrm{d}s\left\langle u_i'(\mathbf{x},t)\nabla\cdot\mathbf{v}_\mathrm{p}(\mathbf{x},t\mid s)\right\rangle - \tau_\mathrm{p}\frac{\partial\overline{v_j'v_i'}}{\partial x_j} \tag{4.25}$$

So it is clear that the momentum equation can be interpreted as a simple ADE equation if the inertial acceleration term on the RHS of Eq. (4.23) is small compared with the gradient diffusion term, and the local value of the particle velocity covariance $\overline{v_i'v_j'}$ has its local homogeneous value: [3] in this case the value of the diffusion coefficient ϵ_{0ij} is given by

$$\epsilon_{0ij} = \int_0^t \langle u_i'(\mathbf{x},t)u_j'(\Delta\mathbf{x}(\mathbf{x},t\mid s),s)\rangle\,\mathrm{d}s \tag{4.26}$$

recalling that in a uniform sheared carrier flow $\Delta\mathbf{x}(\mathbf{x},t|s)$ depends upon the shearing of the carrier flow (Reeks, 1993). In the case of particle deposition models in turbulent pipe flow, the relevant mass flux is that normal to the wall, so the relevant diffusion coefficient is independent of the shearing and appropriate for diffusion in homogeneous turbulence in which the mean carrier flow is spatially uniform.

[3] We mean here that the turbulence is homogeneous and the mean carrier flow is either spatially uniform or with a uniform mean shear.

The conditions are in general

$$\frac{\tau_p\langle u\rangle}{L_u} \ll 1 \quad \frac{\tau_p^2\sigma_0^2}{L_\sigma^2} \ll 1 \quad \frac{\tau_p\epsilon_0}{L_\rho^2} \ll 1 \tag{4.27}$$

where σ_0 is the particle rms velocity as if the turbulence was locally homogeneous and L_u, L_ρ, L_σ are the length scales for variations in mean carrier flow velocity, particle concentration and local homogeneous particle rms velocity σ_0, i.e. more explicitly

$$L_u \sim \frac{\mathrm{d}}{\mathrm{d}x}\ln\langle u\rangle; \quad L_\rho \sim \frac{\mathrm{d}}{\mathrm{d}x}\ln\rho; \quad L_{\sigma_0} \sim \frac{\mathrm{d}}{\mathrm{d}x}\ln\sigma_0 \tag{4.28}$$

The first condition in (4.27) is the condition for particles to follow the mean carrier flow (in the absence of the turbulence); the second condition is for a drift velocity to be given by Eq. (4.25) with the particle velocity covariance given by σ_0^2—this also means that the diffusion coefficient ϵ_0 is given by the form in Eq. (4.26) and the last condition is for gradient diffusion with a diffusion coefficient given by ϵ_0. $\tau_p\langle u\rangle$ is generally referred to as the particle stop distance whilst the length scales $\tau_p\sigma_0$ and $\sqrt{\tau_p\epsilon_0}$ are equivalent to the particle mean free paths λ_σ, λ_ρ for changes in particle velocity and concentration respectively. If $\tau_f(p)$ is the integral timescale of the carrier flow turbulence along a particle trajectory p, and the velocity correlation of the carrier flow is an exponential decay, then using the homogeneous forms for σ_0 and ϵ_0,

$$\begin{aligned} \lambda_\rho &= \sqrt{\tau_p\tau_f(p)}\langle u'^2\rangle^{1/2} \\ \lambda_{\sigma_0}/\lambda_\rho &= (1+\tau_f(p)/\tau_p)^{-1/2} \end{aligned} \tag{4.29}$$

We note therefore that the particle mean free path for changes in particle velocity is always less than that for changes in particle concentration but that in the limit of $\tau_p/\tau_f(p)\to\infty$ both length scales approach the same value (see Fig. 1. For deposition in a turbulent boundary layer the restriction on L_{σ_0}, i.e. upon the gradients of the turbulent intensity and length scale, is the most important criterion on the influence of the fluid motions in the boundary layer itself on whether a simple ADE is appropriate. So noting that L_σ is the same as that for the carrier flow L, and that $L/\sqrt{\langle u'^2\rangle} \sim \tau_{fE}$ where $\tau_{fE}(x)$ is the Eulerian integral timescale of the carrier flow, and using the relationships for λ_{σ_0} and λ_ρ in Eq. (4.29), the second criterion in Eqs. (4.27), reduces to:

$$\left(\frac{\tau_p}{\tau_{fE}}\right)\left(\frac{\tau_f(p)}{\tau_{fE}}\right) \ll 1 \tag{4.30}$$

In the absence of gravity (zero crossing trajectories) the ratio $\tau_{p,f}/\tau_{fE}$ although dependent on τ_p/τ_{fE}, is typically ~ 1, so that the overall criterion would simply be

$$\left(\frac{\tau_p}{\tau_{fE}}\right) \ll 1 \tag{4.31}$$

Under these conditions it is clear that we can use the expression given by Maxey (1987) for the particle compressibility to first order in τ_p/τ_{fE} so that the drift velocity $\mathbf{v}_d$ has components

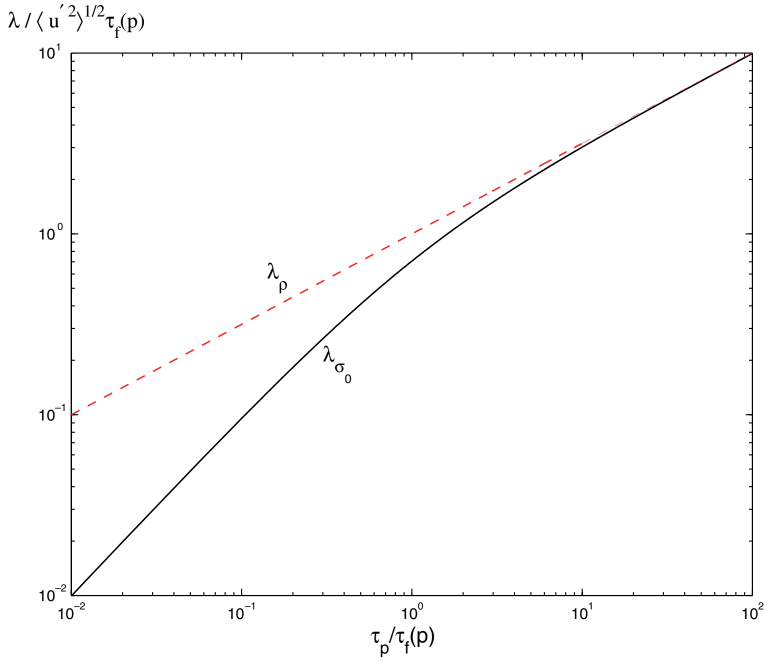

Fig. 1. Particle mean free paths λ_ρ, λ_{σ_0} for changes in particle concentration ρ and particle rms velocity σ_0 respectively.

$$v_{\mathrm{d}_i} = \frac{\tau_\mathrm{p}}{4}\int_0^t \mathrm{d}s\left\langle u_i'(\mathbf{x},t)\left\{\sum_{j,k} S_{jk}^2(\mathbf{x},t\mid 0) - \omega^2(\mathbf{x},t\mid 0)\right\}\right\rangle - \tau_\mathrm{p}\frac{\partial\langle u_i'u_j'\rangle}{\partial x_j} \tag{4.32}$$

where $\mathbf{S}$ and $\underline{\omega}$ are the strain rate tensor and vorticity along the particle trajectory arriving at $(\mathbf{x},t)$ from time zero.

4.2. The influence of boundary conditions

The conditions derived in Eq. (4.27) put restrictions on the spatial variations in the carrier flow field both with regard to its mean and turbulence intensity, i.e. changes in their value must be small over the relevant particle mean free path. Boundary conditions, i.e. whether the containment wall is depositing or reflecting, will also impose restrictions. For instance, suppose we consider a flow which is quasi-homogeneous upto the boundary layer adjacent to a depositing wall for which the conditions in Eq. (4.27) mean that simple gradient diffusion would apply. Suppose that the boundary layer is so thin, that it has no effect on the motion of the particles, i.e. gradient diffusion would be considered to apply right upto the wall with a diffusion coefficient given by that in the bulk 'homogeneous' flow. However the natural boundary conditions for a depositing surface would mean that the particle velocity distribution would change from say near Gaussian away from the wall to a half-Gaussian at the wall in a distance of the order of the particle mean free path $\tau_\mathrm{p}\sigma_0$ where σ_0 is the particle rms velocity in the bulk flow. In other words fractional changes of particle velocity $\Delta\sigma/\sigma_0 \sim 1$ will take place over the particle mean free path $\tau_p\sigma_0$: a similar change will apply to the particle concentration. In other words a simple ADE approximation is only appropriate at least one particle mean free path away from the wall. These features are illustrated graphically in Swailes and Reeks (1993) for the solution of the PDF equation for inertial depositing particles in a turbulent boundary layer.

5. Comparison of approaches

Table 1 compares the two approaches in terms of the features that have been discussed and analysed in the previous sections.

5.1. Implementation of ADE approach by Young and Leeming

It is clear from this table, that YL have implemented the ADE approach in a way that is strictly inconsistent with the way it has been derived and can be applied. That is, the closure approximations for the Reynolds stresses/particle velocity covariances (Eq. (2.10)) and dispersive flux $\langle \mathbf{v}'\rho' \rangle$ (Eq. (4.23)) are only appropriate for quasi-homogeneous flow whilst the form of the transport equation for $\langle \mathbf{v}(\mathbf{x},t) \rangle$ used, would imply that these approximations are also valid when the inertial term $\mathrm{D}\langle \mathbf{v}(\mathbf{x},t) \rangle/\mathrm{D}t$ is important. Even under the assumption of quasi-homogeneity, the form for the flux $\langle \mathbf{v}'\rho' \rangle$ has both a diffusive and a convective flux (see Eq. (3.15)) of which only the former is accounted for in the YL and CGS models. Furthermore the only form for $\langle v_i(\mathbf{x},t) \rangle$ compatible with the use of these quasi-homogeneous forms is

$$\langle v_i(\mathbf{x},t) \rangle = \langle u_i(\mathbf{x},t) \rangle - \tau_p \frac{\partial \langle u'_j u'_i \rangle}{\partial x_j} \tag{5.33}$$

YL were well aware of this deficiency, and their reason for using the equation to predict particle deposition in turbulent pipe flow, was their belief that when the inertial term dominates the deposition process, the convective flux will dominate over the diffusive contribution, so whatever form is used for the particle diffusion coefficient it is of no consequence so long as it is consistent with this behaviour. They argue that only in cases where particles almost follow the turbulent fluctuations in the carrier flow, will the diffusive part be greater or comparable to the convective part and in these circumstances the approximations both for the diffusion coefficient and the gradient of particle velocity covariance will be valid. This of course is an assumption specific to the problem of deposition in a pipe—and not a general statement: indeed, at a perfectly reflecting boundary there is at equilibrium, irrespective of particle inertia, a balance of convective (body forces) and diffusive fluxes (gradient of stresses), so ignoring any influence of particle inertia on the particle diffusion coefficient for simple gradient diffusion, could lead to significant errors. Furthermore in the case of high inertia particles, the conditions in Eqs. (4.27) rule out any possibility of the underlying particle velocity field being Gaussian. Thus according to Eq. (3.17) there will be a significant contribution to the diffusive flux from higher order spatial gradients in the mean particle concentration (see Eq. (3.17)) as well as all the relevant diffusion coefficients $D_{ijk\ldots}$ (see Eq. (3.18)) including D_{ij} being dependent on the ratios of λ_σ/L_σ, λ_ρ/L_ρ. So the assumption that

Table 1
Comparison of ADE approach and two-fluid/PDF approach

Property	ADE approach	Two-fluid equations based on PDF approach
Type of average	Ensemble averages of particle velocity field; density weighted for the dispersive velocity $\overline{\mathbf{v}'}$	Particle density weighted
Types of equation	Uncoupled equations: an ADE + transport equation equation for the advection velocity $\langle \mathbf{v} \rangle$	Coupled equations for the mass, momentum and kinetic stresses
Closure approximation (CA)	Diffusive flux is in general a sum of a drift velocity and spatial gradient fluxes $D_{i_1 i_2 \ldots i_n} \frac{\partial^n \langle \rho \rangle}{\partial x_{i_1} \partial x_{i_2} \ldots \partial x_{i_n}}$; Equation for $\langle \mathbf{v} \rangle$ needs CA for $\langle \mathbf{v}'\mathbf{v}' \rangle$ and $\langle \mathbf{v}' \underline{\nabla} \cdot \mathbf{v}' \rangle$	PDF equation requires CA for net velocity viewed by the particle $\overline{u'}$ at $\mathbf{v}$, $\mathbf{x}$
Gaussian process	If displacements $\Delta\mathbf{x}$ are Gaussian, diffusive flux is a simple gradient Boussinesq approximation; only strictly valid in homogeneous turbulence close to equilibrium ($t \to \infty$) with $\langle \mathbf{v} \rangle = \langle \mathbf{u} \rangle$ uniform or simple straining flow in $\mathbf{x}$	For jointly Gaussian Δx, $\Delta\mathbf{v}$ in particle $[\mathbf{v}, \mathbf{x}]$ space, $\overline{u'}$ given by simple gradient approximation; reduces to a simple ADE if spatial variations in ρ and $\mathbf{v}$ small over particle mean free paths; same as the simple ADE obtained by the ADE approach
Boundary conditions	Not natural, depending on a priori knowledge of the velocity distribution at the wall	Handles natural boundary by solving PDF equation at/near the wall (near wall solution) and matching with far wall solution based on solution of two-fluid equations. PDF method crucial to calculating particle deposition
Limit of heavy particles $\tau_p \to \infty$	Equation for $\langle \mathbf{v}(\mathbf{x}, t) \rangle$ dominated by inertial acceleration $\mathrm{d}\langle \mathbf{v} \rangle / \mathrm{d}t$. Dispersive flux $\langle \rho \mathbf{v}' \rangle$ is determined by non-local diffusion coefficients $D_{ijk\ldots}$. D_{ij} in general $\gg$ quasi homogeneous value $\langle \rho \mathbf{v}' \rangle$ may be same order as convective flux	Particle motion equivalent to Markov process with a white noise driving force. PDF equation reduces to a classical Fokker–Planck equation which describes particle transport exactly
Accuracy and reliability	Probably quite reliable for small particles; could also be accurate for large particles; suffers from lack of closure approximation for $\tau_p/\tau_f(\mathrm{p}) \sim 1$; best suited to calculating particle deposition in pipe-flow, but unsuitable as a general approach	Based on a rational approach. Gaussian assumption for practical implementation reliable approximation in phase space for all τ_p. Use of PDF equation direct, means accurate reproduction of particle wall interactions; a basis for a general approach to two-fluid modelling

the convective flux will dominate over the diffusive flux for high inertia particles is not so obvious when one considers the possibility of inertia increasing the value of the particle diffusion coefficients from their quasi-homogeneous value. So the attractiveness of using an ADE approach where the convection velocity is solved separately, is lost because of the absence of any closure approximations to account for the influence of the particle inertia on the particle Reynolds stresses and in turn upon the gradient diffusion process itself.

5.2. Reliability of PDF approach

On the other hand, although the PDF approach leads to a more conventional coupled set of *two-fluid* continuum equations, it is clear from the comparison in Table 1, that there are a number of properties of the two-fluid/PDF approach which makes it more much more reliable. Although we use a simple ADE approximation in the practical implementation of the PDF approach, we use it at the simplest level of the dynamics in which the underlying Liouville equation upon which the PDF equation is based, is a linear equation and so we may have a better chance of success. What it is important to appreciate, is that a simple ADE approximation at this basic level of the dynamics, does not imply a simple ADE for the spatial dispersion process, i.e. for the spatial concentration alone—indeed we have derived the conditions for which it is valid or not valid. The only real concern with the PDF approach is the fact that fluid point dispersion is assumed to be Gaussian (particles following the carrier flow precisely), noting that for this motion, the conditions for simple ADE are always met. We of course would not expect this to be true except in say homogeneous stationary turbulence in the limit of long diffusion times, but the crucial feature of such processes is that they are non-local and at least this *non-localness* is captured in the formulae for the particle diffusion coefficients etc.

6. Diffusion in a simple inhomogeneous turbulent flow

In this section we illustrate some of the basic features of the ADE and PDF approaches for particle transport in a simple inhomogeneous turbulent flow, i.e. flow with zero or uniform mean flow as is the case for the flow normal to the wall in a turbulent boundary layer. In particular we will consider the dependence of the particle diffusion coefficients as defined in Eqs. (3.15) on the inertial parameter $\tau_p/\tau_f(p)$ and illustrate how the persistence of flow structures related to regions of vorticity and straining, can lead to a significant difference between the particle diffusion coefficient and the fluid point diffusion coefficient. We will also calculate the values for the particle/fluid diffusion coefficient as used in the PDF equation and in the momentum equation and show how accurate it can be calculated by using Eulerian time scales for the fluid point motion seen by the particle.

Thus we consider dispersion in a simple inhomogeneous turbulent flow field composed of pairs of counter rotating vortices which are periodic in both the x, y directions with the same periodicity. Each lattice cell (the basic periodic element) contains a pair of counter-rotating vortices in both the x, y orthogonal directions and is constructed from a linear symmetric straining flow field in the manner shown in Fig. 2. So starting from an initial symmetric straining flow pattern of width $2L$ in both the x, y directions (see Fig. 2(a)), this pattern is repeated *front to back* in both the x, y directions with a strain rate S drawn from a uniform distribution $[0, S_0]$. We note that each quadrant of this straining rate pattern in Fig. 2(a) is a quadrant of one of the two pairs of counter-rotating vortices formed within the lattice cell in Fig. 2(b). As shown in Fig. 3(a), the flow velocity u_x in the x-direction has a linear saw-tooth profile $U(x)$, with a slope of constant magnitude S but with a change in sign across the y-centre line of a vortex [4] where the maximum and minimum

[4] The line running in the y-direction passing through the centre of the vortex.

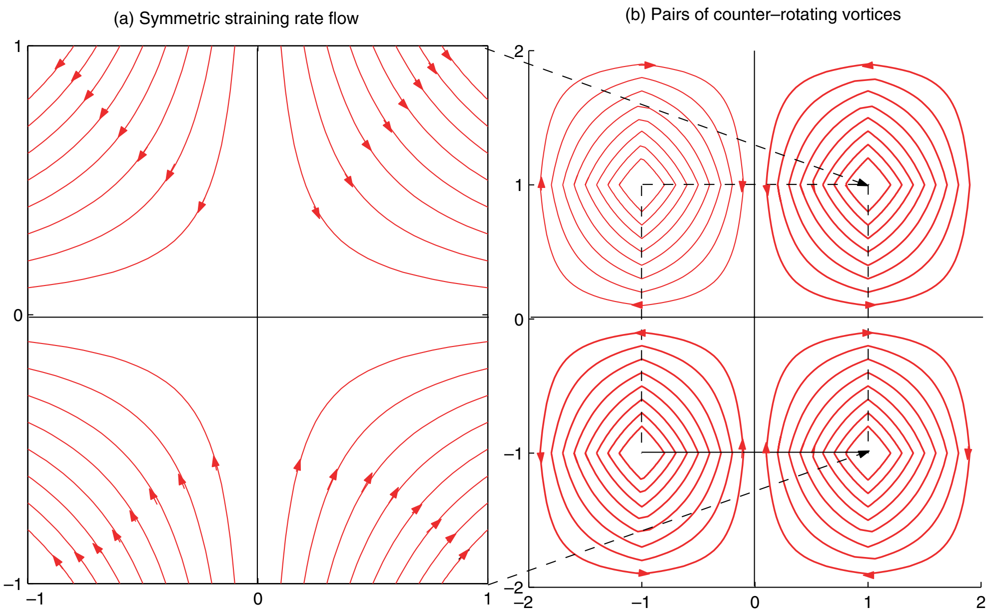

Fig. 2. Generation of flow field used in simulation.

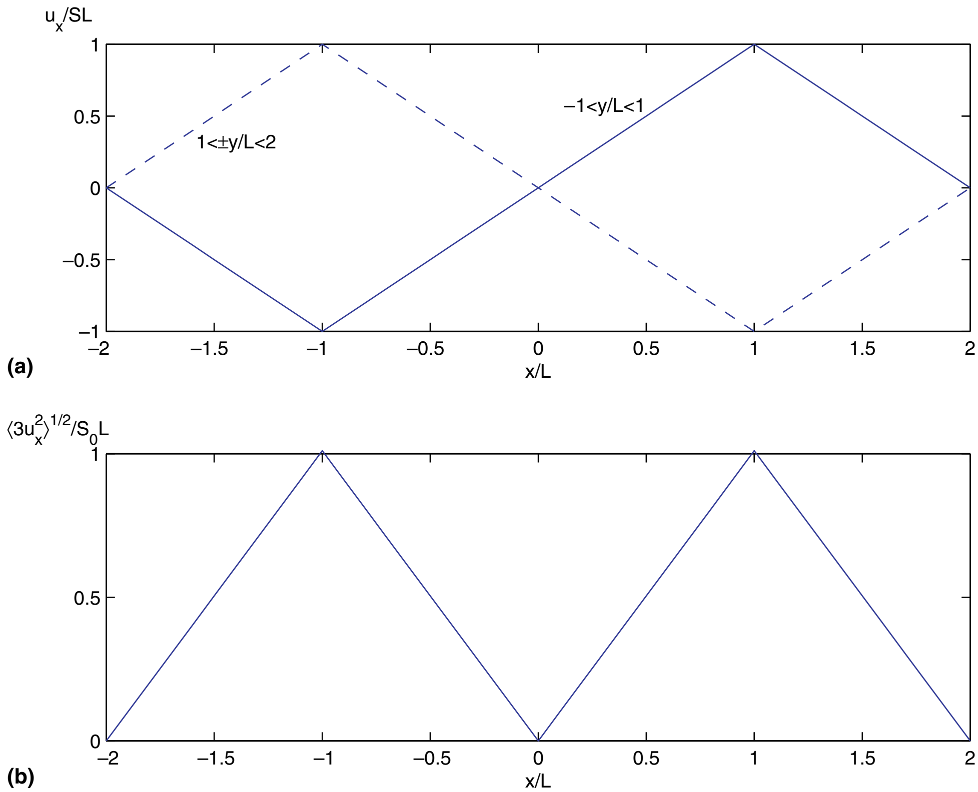

Fig. 3. Flow in x-direction within vortex.

values $\pm SL/2$ of $U(x)$ are located: across the x-centre line, u_x changes to $-U(x)$ as shown in Fig. 3, consistent with the change in direction of the streamlines shown in Fig. 2(b). The flow velocity u_y in the y-direction at (x,y) is $-U(y)$ to preserve continuity of flow through out. This cellular flow pattern of counter-rotating vortices so formed, persists for a fixed life-time selected from an exponential distribution with a decay time of S_0^{-1}, at the end of which time, a fresh flow field is generated with new values of the life-time and S and the origin of the pattern at the same time shifted by a random displacement in the y-direction, drawn from a uniform distribution $[0,2L]$. This makes the average flow homogeneous with zero mean in the y-direction but inhomogeneous in the x-direction. In particular, as shown in Fig. 3(b), the carrier flow rms velocity $\langle u_x^2\rangle^{1/2}$ in the x-direction is a linear saw-tooth in x with a peak value of $S_0L/\sqrt{3}$ along the y–vortex centre lines. The important feature of this randomized flow field is that the equations of motion of an individual particle in both the x, y-directions are linear and independent of one another (other than through the maximum length of time a particle can experience a particular value of the straining of the flow in either the x- or y-directions before it changes sign). With respect to the centre (stagnation point) of a symmetric straining flow pattern (see Fig. 2(a)), the flow velocity within that flow region is given by:

$$u_x = +Sx; \quad u_y = -Sy \quad (-L \leqslant x \leqslant L,\ -L \leqslant y \leqslant L) \tag{6.34}$$

and the particle equation of motion based on Stokes drag, is

$$\ddot{x}_i + \tau_p^{-1}\dot{x}_i + (-1)^{i+1}\tau_p^{-1}Sx_i = 0, \quad (i = 1,2)\ (x_1 = x, x_2 = y) \tag{6.35}$$

where x_i is measured from a stagnation point. For convenience we express the particle response time τ_p in units of S_0^{-1} so S here is strain rate in units of S_0, and picked from a uniform distribution $[0,1]$.

Fig. 4 shows the evaluation of the carrier flow fluid point diffusion coefficient as a function of time for a number of equally spaced locations in x measured from the $x = 0$ stagnation point. The diffusion coefficient is symmetric about a stagnation point $x = 0$ for $-L \leqslant x \leqslant L$, with the pattern repeated periodically over a length scale of $2L$, as is the case for the carrier flow rms etc. (see Fig. 3(b)). Thus in this case, as also in subsequent cases, we only show the values of averaged quantities for $0 \leqslant x \leqslant L$. In this respect therefore the flow in this limit corresponds to a turbulent boundary layer $0 \leqslant x \leqslant L$ with a perfectly reflecting wall at $x = 0$. The significant feature of the fluid point (carrier flow) diffusion coefficient is that whilst rising to peak value at $tS_0 \sim 1$, it tends to zero in the limit of $tS_0 \to \infty$, i.e. the fluid point motion is contained in closed orbits (trapping) so that no matter what the randomness, the basic periodicity of the flow pattern means that the fluid point is confined (i.e. zero diffusion). In other words the actual timescale/length scale for diffusion in the long-term limit is zero ($\tau_f(p) = 0$).

The same procedure of calculating backwards in time t from a given location x cannot be used for particles with inertia $\tau_p > 0$ since we do not know what distribution of velocities to select the particle velocity at say x,t. So in these cases we are forced to track forwards in time from a uniform spatial distribution of particles with some prescribed distribution of velocities: in this case we chose an initial particle velocity distribution identical to that of the carrier flow. Thus is each realisation of the flow, the same particle is introduced randomly into a lattice cell within the

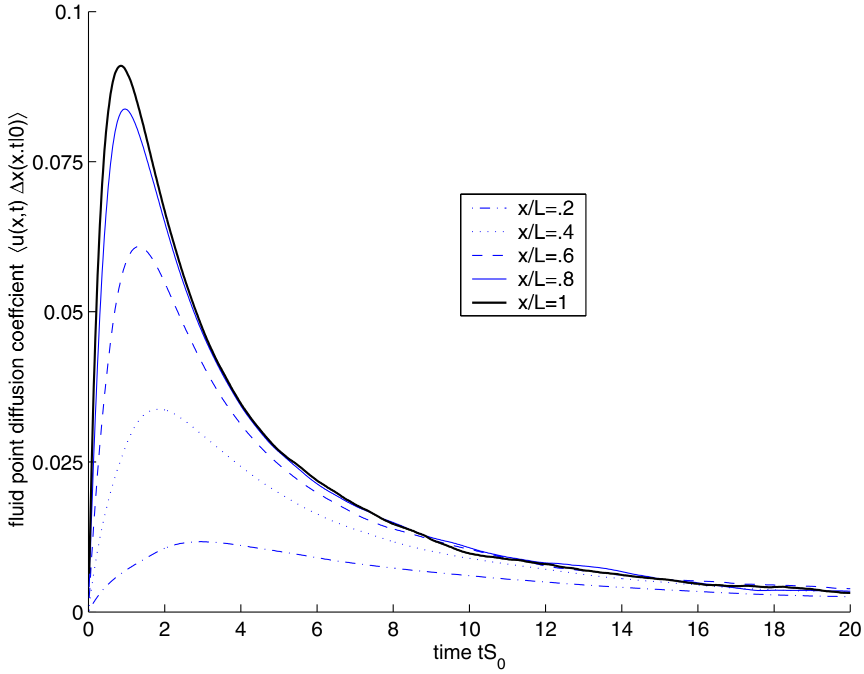

Fig. 4. Fluid–point diffusion as a function of x (distance from y-stagnation line) for random periodic array of counter-rotating vortices.

range $-L \leqslant x \leqslant L$ with a velocity identical to the carrier flow at its x-location. The particle is then tracked by solving the particle equations of motion, Eq. (6.35). At any selected time t, the position within a lattice cell is evaluated with respect to the appropriate stagnation point for which $-L \leqslant x \leqslant L$. By dividing the range $-L \leqslant x \leqslant L$ into a number of consecutive intervals/bins, the particular bin into which the particle location falls is determined, and in turn the displacement of the particle with respect to its initial position $\Delta x(x, t|0)$ is stored along with the particle velocity and carrier flow velocity at x. Although a particle may be tracked beyond the lattice cell within which it was initially located, because of the periodicity of the flow pattern, the statistics or averages determined from the values stored in the bin are the same for the same location in any lattice cell, given that the whole infinite flow domain is seeded uniformally with particles.

As time progresses, the particles are no longer uniformally distributed, but show a distinct build up of concentration in the vicinity of the stagnation point $x = 0$. The behaviour is consistent with a combination of drift and diffusion acting in opposite directions. This build up of concentration increases with time and is dependent upon the value of τ_p. Fig. 5 shows the maximum occurring around $\tau_p \sim 1$.

Figs. 6 and 7 show the spatial dependence of both the particle diffusion coefficient and fluid–particle diffusion coefficient at various increasing times for particles with $\tau_p = 1$. In the case of the particle diffusion coefficient, it is worth noting that its value is not zero at the stagnation point: this is entirely due to the influence of particle inertia or *overshooting* of the particle velocity. In fact

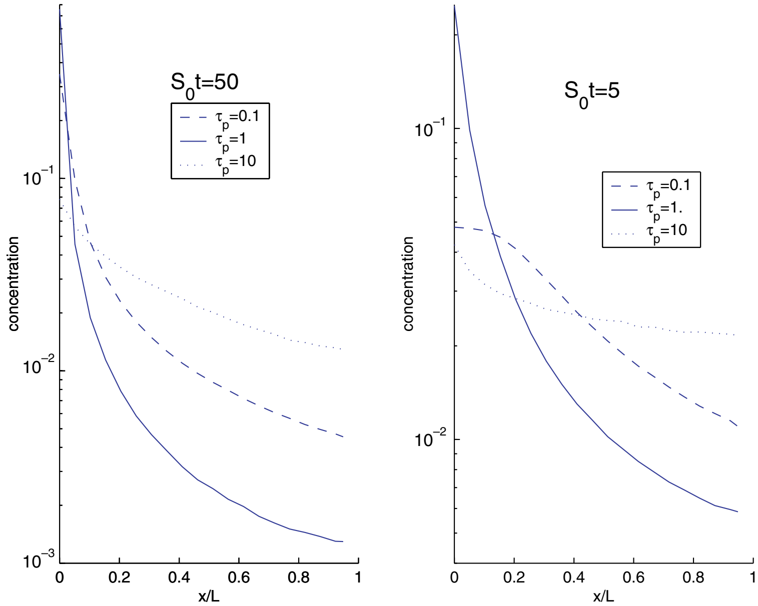

Fig. 5. Concentration profiles at various times and particle response time.

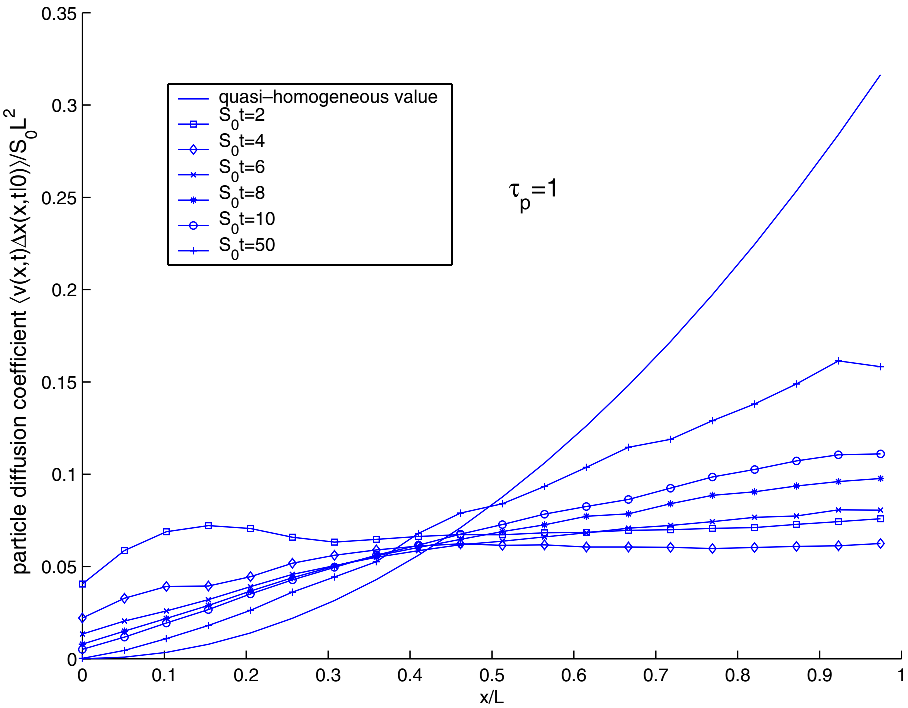

Fig. 6. Particle diffusion coefficient for particles with $\tau_p = 1$, as a function of x (measured from stagnation point) for increasing values of time.

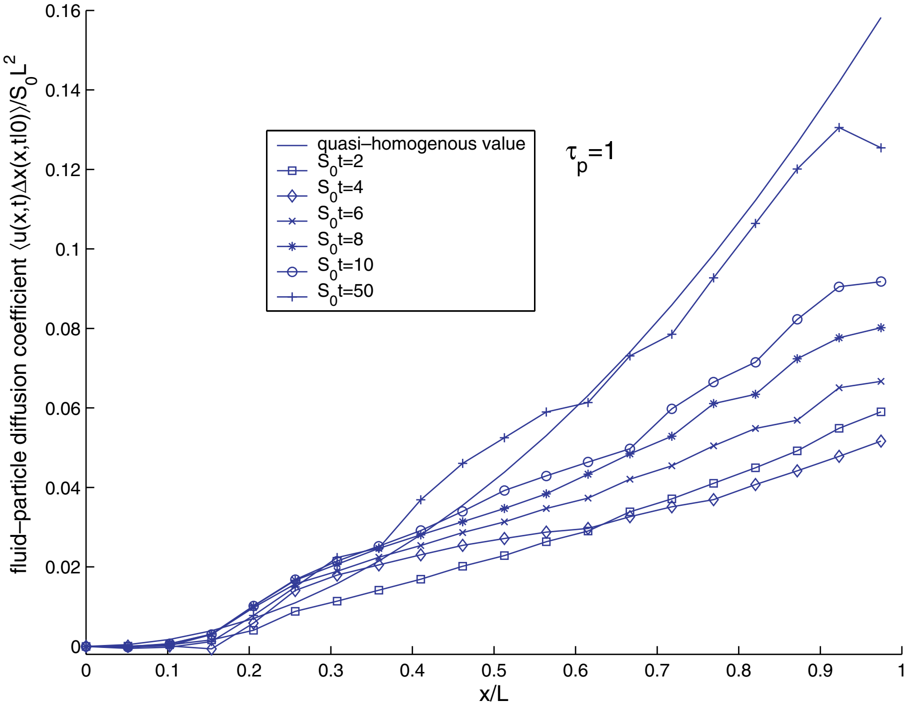

Fig. 7. Fluid–particle diffusion coefficient particles with $\tau_p = 1$, as a function of x (measured from stagnation point) for increasing values of time.

the particle behaviour in this region is very much like a lightly damped harmonic oscillator (critical damping occurring at a value of $\tau_p = 0.25$). The profile at $S_0t = 50$ approximates to the long term values for the particle diffusion coefficient. Compare this with the long term quasi-homogeneous values with $\tau_f(p) = S_0^{-1}$ shown also in Fig. 6 which is independent of particle inertia and given by

$$\langle v_i'(\mathbf{x}, t)\Delta\mathbf{x}_j(t)\rangle_{t\to\infty} = \frac{1}{3}S_0x^2 \tag{6.36}$$

Note that the long term particle diffusion coefficient is less than the corresponding long term quasi-homogeneous value, with a flatter profile. The corresponding values for the fluid–particle diffusion coefficient do not exhibit any influence of overshooting, its value at the stagnation point being always zero. The strict uncertainty in determining its value analytically is the uncertainty of the timescale of the carrier flow turbulence seen by the particle which as we have seen differs significantly between trapped and non trapped particles. For comparison we have shown the long term equilibrium value of this coefficient using the same value for $\tau_f(p)$ as that of the average lifetime of the flow pattern namely S_0^{-1}. So in this case for an exponential correlation of carrier flow velocities seen by the particle,

$$\langle u_i'(\mathbf{x}, t)\Delta\mathbf{x}_j(\mathbf{x}, t \mid 0)\rangle_{t\to\infty} = \frac{1}{3}(1+\tau_p)^{-1}S_0^2x^2 \tag{6.37}$$

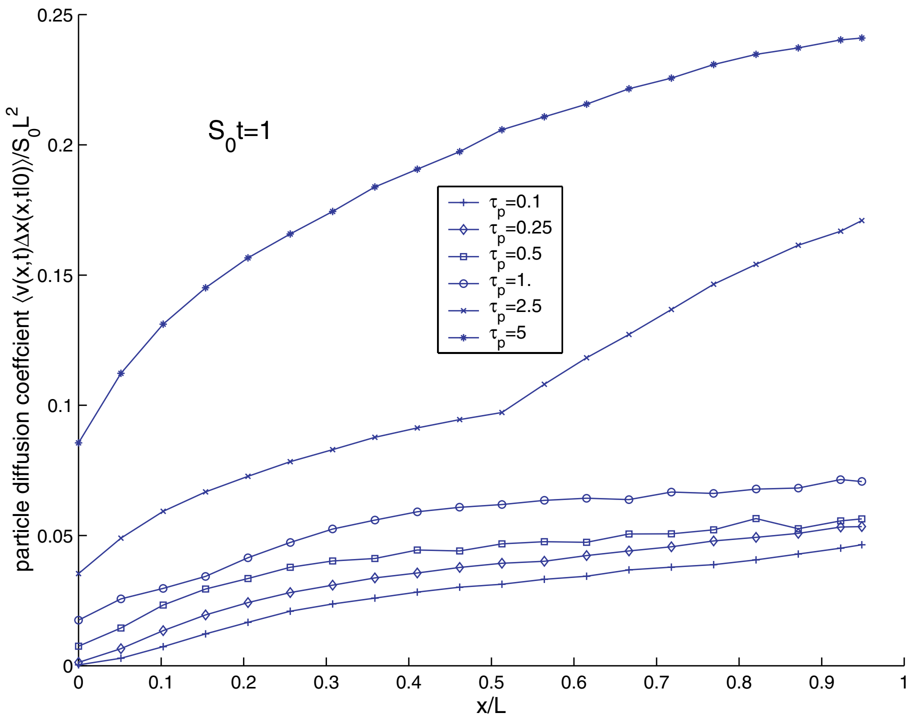

Fig. 8. Particle diffusion coefficient as a function of x (measured from stagnation point) for range of values of particle response times at a fixed time of $S_0t = 1$.

where τ_p is in units of S_0^{-1}. For the case of $\tau_p = 1$ shown, the agreement between this value and the longer term value at $S_0t = 50$ calculated from the simulation is quite good considering the uncertainties in the value of $\tau_f(p)$. Figs. 8 and 9 show the dependence of these same diffusion coefficients upon particle inertia τ_p for a fixed time $tS_0 = 1$. Note that the overshooting in the particle diffusion coefficient due to particle inertia is present only for $\tau_p \geqslant 0.25$ consistent with the behaviour of lightly damped harmonic oscillator: for all values of the particle inertia, the trend is towards increasing particle diffusion coefficient with increasing inertia. For the fluid–particle diffusion coefficient in Fig. 9, there is again no overshooting, and the trend of decreasing value with increasing particle inertia is the same as that for the quasi-homogeneous values, however we note that the values for $\tau_p = 1$ are an exception. The results shown in Fig. 10 show that the long term value of the particle–fluid diffusion coefficient averaged over $0 \leqslant x \leqslant L$ approaches the long term quasi-homogeneous value for large inertia particles. Here the long term value is taken to be at least $S_0t = 10\tau_p$. The average value is chosen for reasons of presentation/accuracy (especially in the case of particles with $\tau_p \gg 1$ where the diffusion coefficient is very small). Such behaviour, as we have stated previously, is consistent with the fact that in this limit of high particle inertia the relevant closure approximation is an exact in the PDF approach, and that the local Eulerian timescales can be used for the timescale of the carrier flow seen by the particle.

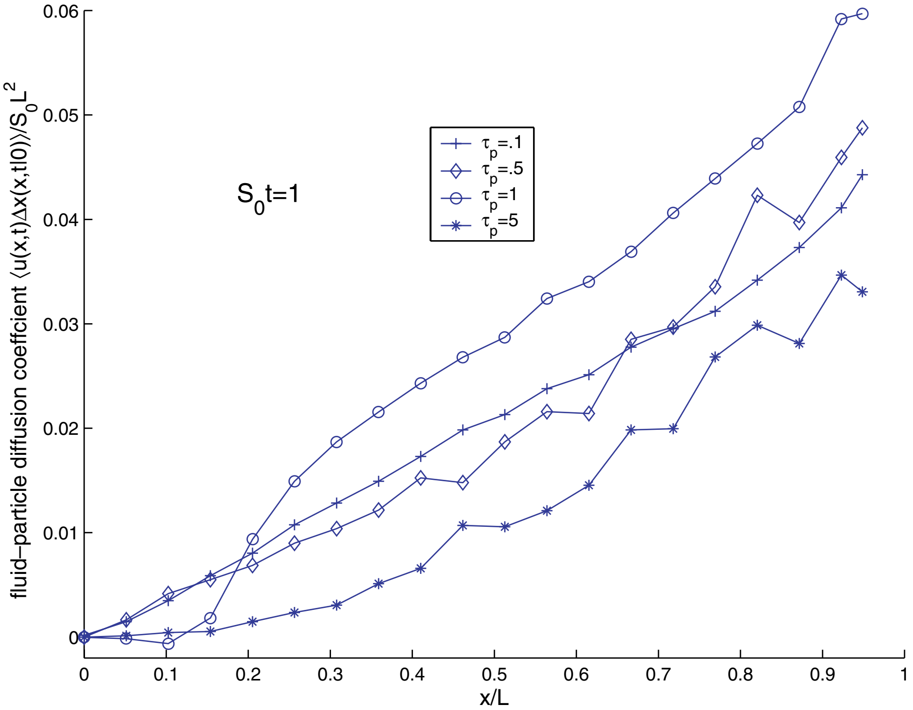

Fig. 9. Fluid–particle diffusion coefficients as a function of x (measured from stagnation point) for range of values of particle response times at a fixed time of $S_0t = 1$.

7. Summary and conclusions

The ADE approach introduced by Young and Leeming to calculate particle deposition in a turbulent layer represents a significant advance in modelling, reproducing the known features of the deposition curve in a simple direct way without resorting to any adjustable constants. Its advantage over that of the traditional two-fluid approach is a strictly computational one however, namely the equation for the mean convective velocity $\langle \mathbf{v} \rangle$ is independent of the equation for the mean particle concentration and mass flux, so $\langle \mathbf{v} \rangle$ can be solved for separately before it is introduced explicitly into the ADE for the mass flux $\langle \rho \mathbf{v} \rangle$. However we have shown that problems arise with the practical application of the ADE in situations where particle inertia $\tau_p/\tau_f(p)$ is important. Whilst the inertial acceleration term $D\langle \mathbf{v} \rangle/Dt$ is directly included in the equation for the local mean particle velocity field, the closure approximations for the drift due to the gradients of kinetic stress (the so called turbophoretic term) and the particle diffusion coefficient both assume forms which are appropriate only for local homogeneous flows and for low inertia particles, i.e. the influence of particle inertia (due to spatial inhomogeneity of the turbulence) is ignored. An analysis of passive scalar dispersion in a compressible flow field leads to a simple ADE only if the flow field is strictly Gaussian which is only justified when changes in the concentration and particle velocity covariance are small over a particle mean free path (see Eq. (4.27))—in this case the ADE reduces to the quasi-homogeneous form. That is the influence of particle inertia is to turn a simple ADE

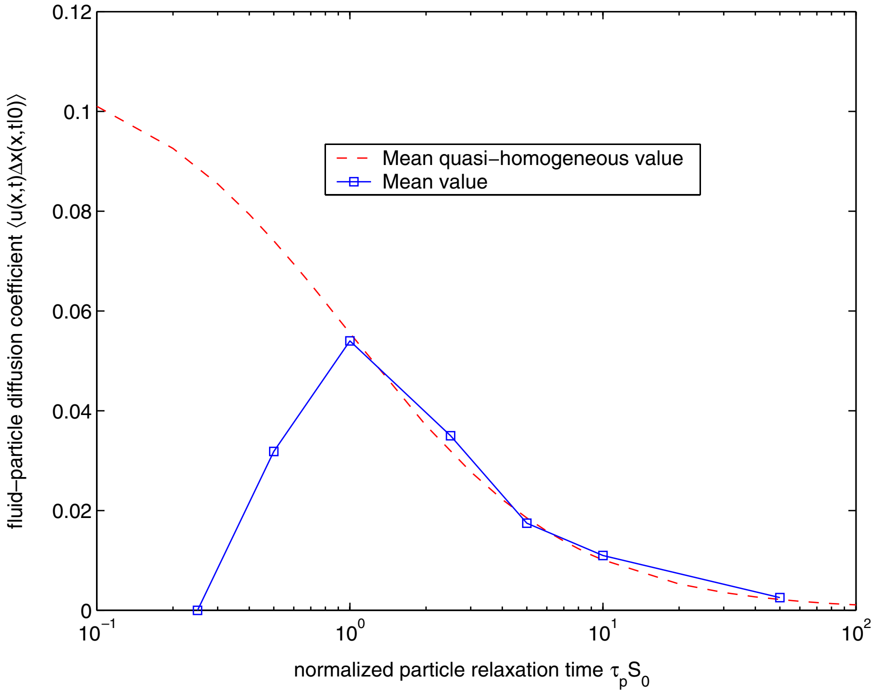

Fig. 10. Fluid–particle diffusion coefficient averaged over $0 \leqslant x \leqslant L$ as a function of particle inertia $\tau_p S_0$.

into one in which the dispersive flux $\langle \rho' \mathbf{v}' \rangle$ depends upon higher order gradients of the mean concentration and diffusion coefficients $D_{ijk\ldots}$ which themselves depend upon the particle inertia and are markedly different from the local homogeneous values.

Furthermore any attempt at using closure approximations borrowed from those for density weighted averages (as in the two-fluid approach), though expedient, is strictly not legitimate and destroys the independence of the equation for the convection and the reason for using an ADE approach in the first place. For consistency all closure approximations in an ADE should be derived from the equation for the particle velocity field, i.e. not involving mean concentration gradients etc.

In Section 5 we gave a number of reasons why the PDF approach was much more reliable than the ADE approach, the most important one being that closure approximations are applied to a linear equation, the Liouville equation, in particle phase space so that simple gradient (Gaussian) approximations have a greater chance of success: certainly the resulting mass–momentum and energy equations admit all the features of a non-Gaussian process even though the underlying process in phase space maybe be Gaussian. Furthermore in the simple inhomogeneous flow considered, the fluid–particle diffusion coefficient used in the PDF approach is much better predicted than the corresponding particle diffusion coefficient using a local homogeneous assumption: what is perhaps even more important is that the approximation gets better the greater the particle inertia and in the limit is exact. Of course the other important and crucial reason for using the PDF approach not touched upon here is that the approach handles natural boundary conditions without any further ad hoc assumptions as in Swailes and Reeks (1993) and Reeks and Swailes (1997).

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