J. Fluid Mech. (2005), *vol.* 522, *pp.* 263–302.
DOI: 10.1017/S0022112004001922 Printed in the United Kingdom

On probability density function equations for particle dispersion in a uniform shear flow

By MICHAEL W. REEKS

School of Mechanical and Systems Engineering, Stephenson Building, University of Newcastle, Newcastle upon Tyne, NE1 7RU, UK
mike.reeks@ncl.ac.uk

(Received 2 December 2003 and in revised form 17 August 2004)

The paper examines a fundamental discrepancy between two probability density function (PDF) models, the kinetic model (KM) and generalized Langevin model (GLM), currently used to model the dispersion of particles in turbulent flows. This discrepancy is manifest in particle dispersion in an unbounded simple shear flow where model predictions for the values of the streamwise fluid-particle diffusion coefficients are not only different but are of opposite sign. It is shown that this discrepancy arises through a neglect of the inertial convection term in the GLM equation for the mean carrier flow velocity local to a particle which eventually leads to algebraic forms for the particle-fluid diffusion coefficients. Evaluating this term for a Gaussian process leads to identical results for both PDF formulations. This also resolves a fundamental long-standing discrepancy in previous forms reported for the passive scalar diffusion coefficients in a simple shear flow where similar assumptions were made. Avoiding this assumption, the exact solutions are given for the dispersion of particles in this simple shear flow case derived from the solution of the GLM PDF equation which show explicitly the dependence on the particle response time and the strain rate, both normalized on the integral timescale of the turbulence. The analysis shows that the particle diffusion coefficient in the streamwise direction is negative when the strain rate $\geqslant$ a certain value. The origin of negative diffusion coefficients is explained and their influence is shown in the way in which the mean concentration and mean velocity flow fields of the particle and carrier flow (seen by the particle) evolve with time for particles released from the centre of the shear.

1. Introduction

The probability density function (PDF) approach is a rational approach to modelling dispersed particle flows in the same way that the kinetic theory is a rational approach for modelling gas flows. That is, there exists in both cases an underlying equation (a master equation) which, in a strictly formal way, can be used to derive both the continuum equations and constitutive relations of a gas or a dispersed phase of particles. In kinetic theory, the master equation is the well-known Maxwell–Boltzmann equation, whilst in dispersed flows, it is known as the PDF equation. There are currently two forms of the PDF equation. In the first form, the PDF, as in kinetic theory, refers to the probability density that a particle has a certain velocity and position at a given time. We will refer to this PDF approach as the kinetic model (KM) approach. This approach was originated by Buyevich (1971, 1972 *a*, *b*) and developed since by a number of workers, most notably Reeks (1980, 1991, 1993), Hyland, Reeks & McKee (1999*a*), Swailes & Darbyshire (1997), Derevich & Zaichik (1988), Zaichik (1991) and Pozorski & Minier (1998). In contrast, the second form of the equation, first proposed by Simonin, Deutsch & Minier (1993, referred to herein as SDM) is for a more general PDF which in addition to the particle velocity and position, includes the velocity of the carrier flow local to the particle.

In the KM approach we use the equation of motion of the particle itself, whilst in the alternative approach we require an additional equation of motion for the carrier flow velocity local to the particle. Currently this latter equation is a simple derivative of the Langevin model used by Pope (Haworth & Pope 1986 and Pope 1994) to describe the motion of the carrier flow velocity itself. Since this method uses a generalized Langevin model for the carrier flow velocity, we shall refer to it here as the GLM approach. As they stand, both approaches will, in principle, give the same results. That is, integrating the GLM PDF equation over all carrier flow velocities local to the particle will yield a kinetic equation which is the same as the kinetic equation in the KM approach. However if the closures used for the unknown terms in either form of PDF equation are incompatible with one another, then this will not happen. Compatibility will only arise if the statistics of the process are the same in either case and the closure is exact in either PDF equation.

The closure approximation used in the KM approach is exact if the carrier flow velocity seen by the particle is derived from a Gaussian process. So the GLM approach will give the same kinetic equation if the closure approximation is exact for the Langevin model and the Langevin equation generates Gaussian statistics for the carrier flow velocity local to the particle. Such a case would be the dispersion of particles in a simple shear flow. In this case the fluxes associated with the carrier flow velocities are linear in the mean particle concentration gradient, thus defining a set of (carrier) fluid-particle diffusion coefficients which contract to the so-called fluid point diffusion coefficients when the particle follows the flow precisely. However the particle diffusion coefficient computed by SDM for the GLM are fundamentally different from those given by the KM approach, showing a different dependence upon the shearing of both phases. This difference, in fact, reflects a long-standing problem in the different values quoted by Rogers, Mansour & Reynolds (1989) and Tavoularis & Corrsin (1985) for the long-term diffusion coefficients for passive scalar (fluid point) dispersion in a simple shear flow.

The purpose of this paper is twofold. First it is to resolve the differences between the approaches. Secondly it is to provide solutions to the dispersion of particles in a simple unbounded shear flow. In this regard we will consider the use of the SDM model equation for the carrier flow velocity encountered by a particle in the shear and solutions will be based on the GLM form of the PDF equation. Whilst particle dispersion in a simple shear has been considered before using the KM approach (Hyland, Reeks & McKee 1999*b*; Swailes, Derbyshire & Reeks 1995; Reeks 1993), the carrier and dispersed phases together did not form a closed system in the sense that the statistical properties of the carrier flow along a particle trajectory were prescribed as inputs assumed independent of the particle motion. In the GLM approach these properties are bound up in the equations of motion themselves (for both particle and carrier flow) and can be extracted as exact analytic solutions of the PDF equations in the case of uniform shear flow.

In § 2 we give a brief description of the KM and GLM approaches. Then in § 3 we use these equations to obtain the transport equations for the mass, momentum and kinetic (Reynolds) stresses of the dispersed phase (the so-called continuum equations) and identify the terms in these equations that require closure. The closure approximations currently used in KM and GLM are given in § 4. Then in § 5, we re-evaluate the closure terms for the case of dispersion of particles in a simple shear and show that, in reality, there is no conflict between the two approaches, identifying, in the process, the source of the error which lead to the apparent inconsistency. In the next section, solutions for the dispersion of particles in a simple shear flow are given, where, in particular, we show how the dispersion scales with time and in what way it depends upon the particle inertia (Stokes number) and the strain rate normalized on the integral timescale of the carrier flow turbulence. Finally in § 7, in the light of the analyses presented, we re-examine the previous work on passive scalar diffusion and consider the legitimacy of the assumptions that lead to the conflict between the various forms of the passive scalar diffusion coefficients.

2. Basic method

We consider an ensemble of identical particles. The velocity and position of an individual particle at time t we denote by $\boldsymbol{v}$ and $\boldsymbol{x}$ respectively. At $\boldsymbol{v}, \boldsymbol{x}$ at time t, the carrier flow velocity is denoted by $\boldsymbol{u}$. The particle is subject to a drag force dependent on the relative velocity $\boldsymbol{v} - \boldsymbol{u}$. The particle equation of motion is thus:

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{v}, \tag{2.1}$$

$$\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \boldsymbol{\beta}\cdot(\boldsymbol{u} - \boldsymbol{v}), \tag{2.2}$$

where $\boldsymbol{\beta}$ is the particle inverse response time tensor. As in SDM and elsewhere, we assume that $\boldsymbol{\beta}$ is a function of the mean of $|\boldsymbol{v} - \boldsymbol{u}|$. The elements of $\boldsymbol{\beta}$ are inverse particle response times which in the case of Stokes drag are constants of the motion. To the particle equations of motion we add an equation of motion of the carrier flow velocity $\boldsymbol{u}$ along the particle trajectory, namely

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = F_i(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t). \tag{2.3}$$

In the first approach, we consider continuum equations derived from an equation for the phase-space density $W(\boldsymbol{v}, \boldsymbol{x}, t)$ in which $\boldsymbol{u}(\boldsymbol{x}, t)$ is a random function of $\boldsymbol{x}, t$, and $\boldsymbol{v}$ and $\boldsymbol{x}$ are independent random variables. In the second approach, the continuum equations are derived from a conservation equation for the phase-space density $P(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t)$ where $\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}$ form a set of independent variables. The transport/conservation equations for $W(\boldsymbol{v}, \boldsymbol{x}, t)$ and $P(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t)$ are respectively

$$\left\{\frac{\partial}{\partial t} + \frac{\partial}{\partial x_i}v_i + \frac{\partial}{\partial v_i}\beta_{ij}(u_j(\boldsymbol{x}, t) - v_j)\right\} W(\boldsymbol{v}, \boldsymbol{x}, t) = 0, \tag{2.4}$$

$$\left\{\frac{\partial}{\partial t} + \frac{\partial}{\partial x_i}v_i + \frac{\partial}{\partial v_i}\beta_{ij}(u_j - v_j) + \frac{\partial}{\partial u_i}F_i(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t)\right\} P(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t) = 0. \tag{2.5}$$

Note that integrating the equation for P over all $\boldsymbol{u}$ gives the equation for W. We resolve $u_i(\boldsymbol{x}, t)$ and $F_i(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t)$ into mean and fluctuating parts:

$$u_i = \langle u_i \rangle + u_i'', \quad F_i = \langle F_i \rangle + F_i'', \tag{2.6}$$

where $\langle \ldots . \rangle$ represents an ensemble average. Then the transport equations for mean values of W and P, namely $\langle W\rangle$ and $\langle P\rangle$, are

$$\left\{\frac{\partial}{\partial t}+\frac{\partial}{\partial x_i}v_i+\frac{\partial}{\partial v_i}\beta_{ij}(\langle u_j\rangle - v_j)\right\}\langle W\rangle = -\frac{\partial}{\partial v_i}\beta_{ij}\langle u_j'' W\rangle, \qquad (2.7)$$

$$\left\{\frac{\partial}{\partial t}+\frac{\partial}{\partial x_i}v_i+\frac{\partial}{\partial v_i}\beta_{ij}(u_j - v_j)+\frac{\partial}{\partial u_i}\langle F_i\rangle\right\}\langle P\rangle = -\frac{\partial}{\partial u_i}\langle F_i'' P\rangle. \qquad (2.8)$$

When suitably normalized $\langle W\rangle$ and $\langle P\rangle$ represent the probability density at time t that a particle has $(\boldsymbol{v}, \boldsymbol{x})$ and $(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x})$ respectively. To solve these equations requires closure relations for $\langle u_i'' W\rangle$ and $\langle F_i'' P\rangle$. For simplicity we shall just deal with the case where $\beta_{ij} = \beta\delta_{ij}$.

2.1. *Closure model for the KM approach*

Based on either the LHDI approximation (Reeks 1993) or the Furutsu Novikov formula (e.g. Swailes & Derbyshire 1997), the closure approximation for the net flux $\langle u_i'' W\rangle$ for particles with velocity $\boldsymbol{v}$ and position $\boldsymbol{x}$ at time t is given by

$$\langle u_i'' W\rangle = -\left(\frac{\partial}{\partial x_j}\langle u_i(\boldsymbol{x},t)\Delta x_j\rangle + \frac{\partial}{\partial v_j}\langle u_i(\boldsymbol{x},t)\Delta v_j\rangle\right)\langle W\rangle - \left\langle \frac{\partial u_i''}{\partial x_j}\Delta x_j\right\rangle\langle W\rangle \qquad (2.9)$$

where explicitly $\Delta x_j(\boldsymbol{x}, \boldsymbol{v}, t|0)$ and $\Delta v_j(\boldsymbol{x}, \boldsymbol{v}, t|0)$ denote changes in the particle position and velocity for a particle starting somewhere in the particle phase space at some initial time $s=0$ and arriving at the point $\boldsymbol{v}, \boldsymbol{x}$ at time $s=t$. The result is exact for a process in which the displacements $\Delta x_j(\boldsymbol{x}, \boldsymbol{v}, t|0)$, $\Delta v_j(\boldsymbol{x}, \boldsymbol{v}, t|0)$ form a Gaussian process. We shall refer to $\langle u_i(\boldsymbol{x},t)\Delta x_j\rangle$ and $\langle u_i(\boldsymbol{x},t)\Delta v_j\rangle$ as the fluid-particle diffusion coefficients for spatial and velocity gradient diffusion respectively in phase space.

2.2. *Closure model for the GLM approach*

SDM derive an equation of motion for the fluid velocity along a particle trajectory by starting from the Langevin equation which Haworth & Pope (1986) have used as the analogue of the Navier–Stokes equation for fluid point motion. Thus along a fluid point trajectory

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \alpha_{ij}(\boldsymbol{x})(\langle u_j\rangle - u_j) + f_i(\boldsymbol{x}) + f_i''(t) \qquad (2.10)$$

where $f_i(\boldsymbol{x})$ is the net viscous and pressure force per unit mass of fluid and $f_i''(t)$ is a white noise function of time.† For future reference we note that

$$f_i(\boldsymbol{x}) = \frac{\mathrm{D}_f\langle u_i\rangle}{\mathrm{D}t} + \frac{\partial\langle u_j'' u_i''\rangle}{\partial x_j} \qquad (2.11)$$

where

$$\frac{\mathrm{D}_f}{\mathrm{D}t} = \frac{\partial}{\partial t} + \langle u_j\rangle\frac{\partial}{\partial x_j}. \qquad (2.12)$$

SDM use this equation to generate an equation of motion for the fluid velocity along a particle trajectory. That is if, as before, $\mathrm{d}/\mathrm{d}t$ is the time derivative along a particle

† Both SDM and Pope consider the equation of motion in differential form because the white noise is assumed non-differentiable. For convenience we have assumed that the white noise here, like all turbulence related functions, is differentiable: it has white noise properties simply because it has a timescale much shorter than the timescale over which $\boldsymbol{u}(t)$ varies along a fluid point $O(\alpha^{-1})$.

trajectory and similarly $\mathrm{d}_f/\mathrm{d}t$ that along a fluid point trajectory, then we have

$$\begin{aligned}\frac{\mathrm{d}u_i}{\mathrm{d}t} &= \left(\frac{\partial}{\partial t} + v_j\frac{\partial}{\partial x_j}\right)u_i(\boldsymbol{x},t)\\ &= (v_j - u_j)\frac{\partial u_i(\boldsymbol{x},t)}{\partial x_j} + \frac{\mathrm{d}_f u_i}{\mathrm{d}t}\\ &= (v_j - u_j)\frac{\partial u_i(\boldsymbol{x},t)}{\partial x_j} + \alpha_{ij}(\langle u_j\rangle - u_j) + f_i(\boldsymbol{x}) + f_i''(t). \end{aligned} \tag{2.13}$$

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

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = (v_j - u_j)\frac{\partial\langle u_i(\boldsymbol{x},t)\rangle}{\partial x_j} + \alpha_{ij}(\langle u_j\rangle - u_j) + f_i(\boldsymbol{x}) + f_i''(t). \tag{2.14}$$

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

$$\begin{aligned}\langle F_i''(\boldsymbol{x},t)P(\boldsymbol{v},\boldsymbol{x},\boldsymbol{u},t)\rangle &= \langle f_i''(t)P(\boldsymbol{v},\boldsymbol{u},\boldsymbol{x},t)\rangle\\ &= -\int_0^\infty \langle f_i''(0)f_j''(s)\rangle\,\mathrm{d}s\frac{\partial\langle P\rangle}{\partial u_j}.\end{aligned} \tag{2.15}$$

Then from equation (2.8), the equation for $\langle P\rangle$ used by SDM is

$$\begin{aligned}&\frac{\partial\langle P\rangle}{\partial t} + \frac{\partial}{\partial x_i}v_i\langle P\rangle + \frac{\partial}{\partial v_i}\beta_{ij}(u_j - v_j)\langle P\rangle\\ &+\frac{\partial}{\partial u_i}\left[\alpha_{ij}(\langle u_j\rangle - u_j) + f_i(\boldsymbol{x}) + (v_j - u_j)\frac{\partial\langle u_i\rangle}{\partial x_j}\right]\langle P\rangle = \int_0^\infty \langle f_i''(0)f_j''(s)\rangle\,\mathrm{d}s\frac{\partial^2\langle P\rangle}{\partial u_i u_j}.\end{aligned} \tag{2.16}$$

3. Continuum equations for the particle phase

These equations refer to the transport of mass, momentum and kinetic stress of the particle phase and can be generated from the PDF equations for $\langle P\rangle$ or $\langle W\rangle$ by multiplying them by an appropriate power of $m\,v'^p v'^q v'^r$ .... and then integrating over all $\boldsymbol{u}$ and $\boldsymbol{v}$ (for $\langle P\rangle$) and over all $\boldsymbol{v}$ (for $\langle W\rangle$) where m is the mass of a particle (assuming for the sake of simplicity that all the particles have the same mass m) and v_i' is the fluctuating value of v_i relative its mean density-weighted value $\bar{v}_i$. Thus

$$\text{mass } \langle\rho\rangle = m\int\langle P\rangle(\boldsymbol{v},\boldsymbol{u},\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{u}, \tag{3.1}$$

$$\text{momentum } \langle\rho\rangle\bar{v}_i = m\int\langle P\rangle(\boldsymbol{v},\boldsymbol{u},\boldsymbol{x},t)v_i\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{u}, \tag{3.2}$$

$$\text{kinetic stress } \langle\rho\rangle\overline{v_i'v_j'} = m\int\langle P\rangle(\boldsymbol{v},\boldsymbol{u},\boldsymbol{x},t)v_i'v_j'\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{u}. \tag{3.3}$$

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

So the quantities $\bar{v}_i$ and $\overline{v_i' v_j'}$ are the particle mass density-weighted mean and covariance of the particle velocities at $(\boldsymbol{x}, t)$. The continuum equations, are from equation (2.7),

$$\frac{\partial\langle\rho\rangle}{\partial t} + \frac{\partial}{\partial x_i}\langle\rho\rangle\bar{v}_i = 0, \tag{3.4}$$

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\bar{v}_i = -\frac{\partial}{\partial x_j}\langle\rho\rangle\overline{v_i' v_j'} + \langle\rho\rangle\beta_{ij}(\langle u_j\rangle - \bar{v}_j) + \beta_{ij}\langle\rho\rangle\overline{u_j''}, \tag{3.5}$$

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{v_i' v_j'} = -\frac{\partial}{\partial x_k}\langle\rho v_k' v_j' v_i'\rangle + \rho\overline{v_j' v_k'}\frac{\partial\bar{v}_i}{\partial x_k} + \langle\rho\rangle\overline{v_i' v_k'}\frac{\partial\bar{v}_j}{\partial x_k} - \langle\rho\rangle\beta_{ik}(2\overline{v_k' v_j'} - \overline{u_k' v_j'} - \overline{v_k' u_j'}), \tag{3.6}$$

where $u_i' = u_i - \overline{u_i}$ and $\mathrm{D}/\mathrm{D}t$ is the particle substantial derivative, i.e.

$$\frac{\mathrm{D}}{\mathrm{D}t} = \frac{\partial}{\partial t} + \bar{v}_j\frac{\partial}{\partial x_j}.$$

So we require closed expressions for:

(i) $\bar{\boldsymbol{u}}''$, the average fluid velocity relative to $\langle\boldsymbol{u}\rangle$ along a particle trajectory;

(ii) $\overline{u_k' v_j'}$, the carrier-particle velocity covariances;

(iii) $\langle\rho v_k' v_j' v_i'\rangle$, the turbulent kinetic energy flux.

Note the distinction here between variables u_i'' and u_i'. Here and throughout we shall use superscripts $''$ and $'$ to refer to random variables relative to $\langle\boldsymbol{u}\rangle$ and density-weighted averages respectively, e.g $\boldsymbol{v}'' = \boldsymbol{v} - \langle\boldsymbol{u}\rangle$; $\boldsymbol{v}' = \boldsymbol{v} - \bar{\boldsymbol{v}}$.

4. Closure of the continuum equations

4.1. *KM approach*

Using (2.7) with (2.9) and suitably integrating it over all particle velocities to form transport equations for the particle-phase momentum and particle kinetic stresses and comparing the resulting equations with (3.5) and (3.6), we obtain the identities

$$\overline{u_i''}\langle\rho\rangle = -\frac{\partial}{\partial x_j}(\langle u_i''(\boldsymbol{x}, t)\Delta x_j(\boldsymbol{x}, t|0)\rangle\langle\rho\rangle) - \left\langle\frac{\partial u_i''}{\partial x_j}\Delta x_j\right\rangle\langle\rho\rangle, \tag{4.1}$$

$$\overline{u_i' v_j'} = \langle u_i''(\boldsymbol{x}, t)\Delta v_j(\boldsymbol{x}, t|0)\rangle - \langle u_i''(\boldsymbol{x}, t)\Delta x_m(\boldsymbol{x}, t|0)\rangle\frac{\partial\overline{v_j}}{\partial x_m}, \tag{4.2}$$

where the displacements $\Delta\boldsymbol{v}$ and $\Delta\boldsymbol{x}$ refer to all particle trajectories arriving at $\boldsymbol{x}$ at time t irrespective of their velocity. $\langle u_i''(\boldsymbol{x}, t)\Delta v_j(\boldsymbol{x}, t|0)\rangle$ is the fluid-particle velocity diffusion coefficient and $\langle u_i''(\boldsymbol{x}, t)\Delta x_j(\boldsymbol{x}, t|0)\rangle$ the fluid-particle spatial diffusion coefficient.

4.2. *GLM approach*

The closure expressions in this case are transport equations for $\overline{\boldsymbol{u}''}$ and $\overline{u_k' v_j'}$ derived from the GLM PDF equation for $\langle P\rangle$, equation (2.16). Multiplying (2.16) by u_i and integrating over all $\boldsymbol{v}$ and $\boldsymbol{u}$ we have

$$\frac{\partial}{\partial t}\langle\rho u_i\rangle + \frac{\partial}{\partial x_j}\langle\rho v_j u_i\rangle = \left\{f_i(\boldsymbol{x}) - \alpha_{ij}\overline{u_j''} + (\bar{v}_k - \bar{u}_k)\frac{\partial\langle u_j\rangle}{\partial x_k}\right\}\langle\rho\rangle. \tag{4.3}$$

Recognizing that we can rewrite the left-hand side as

$$\frac{\partial}{\partial t}\langle\rho u_i\rangle + \frac{\partial}{\partial x_j}\langle\rho v_j u_i\rangle = \langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\langle u_i\rangle + \langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{u_i''} + \frac{\partial}{\partial x_j}\overline{v_j' u_i'}\langle\rho\rangle, \tag{4.4}$$

that from (2.12) and (2.6),

$$\left(\frac{\partial}{\partial t}+\bar{u}_j\frac{\partial}{\partial x_j}\right)\langle u_i\rangle=\frac{\mathrm{D}_f\langle u_i\rangle}{\mathrm{D}t}+\overline{u_j''}\frac{\partial\langle u_i\rangle}{\partial x_j}$$

and using (2.11), gives finally the transport equation for $\overline{u_i''}$, namely

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{u_i''}=-\frac{\partial}{\partial x_j}\overline{v_j'u_i'}\langle\rho\rangle+\langle\rho\rangle\frac{\partial}{\partial x_j}\langle u_j''u_i''\rangle-\left\{\frac{\partial\langle u_i\rangle}{\partial x_j}+\alpha_{ij}\right\}\overline{u_j''}\langle\rho\rangle \tag{4.5}$$

A transport equation can also be obtained for $\overline{u_k'v_j'}$ by transforming the GLM PDF equation into an equation for $P(\boldsymbol{v}',\boldsymbol{u}',\boldsymbol{x},t)$, multiplying the result by $u_i'v_j'$ and then integrating over all $\boldsymbol{u}'$ and $\boldsymbol{v}'$. This gives

$$\begin{aligned}\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{u_i'v_j'}=&-\frac{\partial}{\partial x_k}\langle\rho\rangle\overline{u_i'v_j'v_k'}-\langle\rho\rangle\overline{v_j'v_k'}\frac{\partial\overline{u_i''}}{\partial x_k}\\&-\left(\langle\rho\rangle\overline{u_i'v_k'}\frac{\partial\overline{v}_j}{\partial x_k}+\overline{v_j\prime u_k'}\frac{\partial\overline{u_i}}{\partial x_k}\right)-\langle\rho\rangle\beta(\overline{u_i'v_j'}-\overline{u_i'u_j'})-\langle\rho\rangle\alpha_{ik}\overline{u_k'v_j'}.\end{aligned} \tag{4.6}$$

5. Closure models based on dispersion in a mean uniform-shear flow

The purpose of this section will be to pinpoint the discrepancy in the forms for the fluid-particle diffusion coefficients given by the KM approach in (4.2) and those obtained by SDM by ignoring the inertial acceleration term in (4.5). We then show that if the inertial acceleration term is explicitly evaluated for a Gaussian process, along with the other terms in (4.5), the forms for the fluid-particle diffusion coefficients are compatible with those in the KM approach.

5.1. *KM approach*

In the case of dispersion in a uniform mean flow or a uniform mean shear flow in which the turbulence is homogeneous in both cases, we can express $\Delta\boldsymbol{v}$ and $\Delta\boldsymbol{x}$ in (4.1) and (4.2) in terms of a set of response functions $G_{ji}^{\boldsymbol{x}}(s)$ which are the displacements of the particle in the x_i-direction in response to an impulsive force $\boldsymbol{\delta}(s)$ applied in the $\hat{x}_j$-direction of the mean flow (in the absence of the turbulence). Thus if $\boldsymbol{u}''(s)$ is the fluctuating value of the carrier flow velocity with respect to its mean encountered by a particle along its trajectory measured at time s, then because the mean flow field is linear in $\boldsymbol{x}$,

$$\Delta x_i(t)=\beta\int_0^t u_j''(s)G_{ji}^{\boldsymbol{x}}(t-s)\,\mathrm{d}s,\quad \Delta v_i(t)=\beta\int_0^t u_j''(s)\dot{G}_{ji}^{\boldsymbol{x}}(t-s)\,\mathrm{d}s, \tag{5.1}$$

where $G_{ji}(t)$is the solution of the equation

$$\ddot{G}_{ji}^{\boldsymbol{x}}+\beta\dot{G}_{ji}^{\boldsymbol{x}}-\beta G_{jk}^{\boldsymbol{x}}\frac{\partial\langle u_i\rangle}{\partial x_k}=\delta_{ji}\delta(t). \tag{5.2}$$

So explicitly

$$\left.\begin{aligned}\langle u_i''(\boldsymbol{x},t)\Delta x_j(\boldsymbol{x},t|0)\rangle&=\beta\int_0^t\langle u_i''(\boldsymbol{x},t)u_k''(\boldsymbol{x},t|s)\rangle\,G_{kj}^{\boldsymbol{x}}(t-s)\,\mathrm{d}s,\\\langle u_i''(\boldsymbol{x},t)\Delta v_j(\boldsymbol{x},t|0)\rangle&=\beta\int_0^t\langle u_i''(\boldsymbol{x},t)u_k''(\boldsymbol{x},t|s)\rangle\,\dot{G}_{kj}^{\boldsymbol{x}}(t-s)\,\mathrm{d}s,\end{aligned}\right\} \tag{5.3}$$

with the drift term (the second term on the right-hand side of (4.1)) set equal to zero. In the case of a simple mean shear flow, we have

$$\frac{\partial \langle u_i \rangle}{\partial x_j} = S\delta_{i1}\delta_{j2}. \tag{5.4}$$

The response functions have been derived explicitly for this flow before (Reeks 1993). To distinguish between homogeneous and deviatoric components of the various moments of the PDF distributions, we conveniently split $\boldsymbol{G}^x$ into a corresponding homogeneous component $\boldsymbol{G}^{x(0)}$ and a deviatoric component $\Delta\boldsymbol{G}^x$, i.e.

$$\boldsymbol{G}^x = \boldsymbol{G}^{x(0)} + \Delta\boldsymbol{G}^x \tag{5.5}$$

with

$$\boldsymbol{G}^{x(0)} = \begin{pmatrix} \beta^{-1}(1-\mathrm{e}^{-\beta t}) & 0 \\ 0 & \beta^{-1}(1-\mathrm{e}^{-\beta t}) \end{pmatrix}, \tag{5.6}$$

$$\Delta\boldsymbol{G}^x = S\begin{pmatrix} 0 & 0 \\ \dfrac{1}{\beta}\left\{\dfrac{2}{\beta}(\mathrm{e}^{-\beta t}-1)+t(1+\mathrm{e}^{-\beta t})\right\} & 0 \end{pmatrix}. \tag{5.7}$$

So the corresponding homogeneous and deviatoric components of the phase-space diffusion coefficients in (5.3) are obtained by simply replacing $\boldsymbol{G}^x(t-s)$ in these equations by $\boldsymbol{G}^{x(0)}(t-s)$ and $\Delta\boldsymbol{G}^x(t-s)$ respectively. We note from (5.7) that, in general, the phase-space diffusion coefficients are asymmetric and in particular the deviatoric components of $\langle u_1''(\boldsymbol{x},t)\Delta x_2(\boldsymbol{x},t|0)\rangle$ and $\langle u_1''(\boldsymbol{x},t)\Delta v_2(\boldsymbol{x},t|0)\rangle$ are both zero.†

The forms for $\boldsymbol{G}^x(t)$ given in (5.6) and (5.7) have been used to obtain the long-time values of the dispersion coefficients in the manner of (5.3) using an exponential decay for the Lagrangian carrier flow velocity correlation along a particle trajectory, namely

$$\langle u_i''(t)u_k''(s)\rangle = \langle u_i''u_k''\rangle \mathrm{e}^{-|t-s|/\tau} \tag{5.8}$$

where because of homogeneity we have dropped the dependence of $\boldsymbol{u}''(\boldsymbol{x},t|s)$ on $\boldsymbol{x}$. Recalling explicitly the result for the long-term values as $t\to\infty$, $\langle u_i''(t)\Delta x_j(t)\rangle_\infty$ and $\langle u_i''(t)\Delta v_j(t)\rangle_\infty$ in Reeks (1993), we have

$$\langle u_i''(t)\Delta x_j(t)\rangle_\infty \tau^{-1} = \langle u_i''(t)\Delta v_j(t)\rangle_\infty = \frac{\beta}{\beta+1}\langle u_i''u_j''\rangle_\infty + \delta_{j1}\frac{S\beta^2}{(\beta+1)^2}\langle u_2''u_i''\rangle_\infty \tag{5.9}$$

where both β and S are normalized on τ^{-1}. For the case of $\beta \gg 0$ the result for $\langle u_i''(t)\Delta x_j(t)\rangle_\infty$ corresponds to the diffusion coefficients D_{ij} of a passive scalar in a uniform shear flow, namely

$$\langle u_i''(t)\Delta x_j(t)\rangle_\infty = \tau\langle u_i''u_j''\rangle_\infty + S\tau\delta_{j1}\langle u_2''u_i''\rangle_\infty. \tag{5.10}$$

This is the same as given by Tavoularis & Corrsin (1985). Note that since $\langle u_2''u_1''\rangle \leqslant 0$, equation (5.10) admits the possibility that $\langle u_i''(t)\Delta x_j(t)\rangle \leqslant 0$, a result we shall return to later.

† The homogeneous component should not be confused with the component which is independent of the strain rate because the carrier flow Reynolds stresses (upon which the homogeneous component is linearly related) are themselves dependent upon the local strain rate. Likewise the deviatoric component is not necessarily all of the component proportional to the strain rate.

To obtain the values for the fluid-particle velocity covariances we can use (4.2) which for the simple shear becomes explicitly

$$\overline{u_i'v_j'}_{\infty} = \langle u_i''(\boldsymbol{x},t)\Delta v_j(\boldsymbol{x},t|0)\rangle_\infty - S\tau^{-1}\langle u_i''(\boldsymbol{x},t)\Delta x_2(\boldsymbol{x},t|0)\rangle_\infty \delta_{j1} \tag{5.11}$$

where S has been likewise normalized on τ^{-1}.

Substituting the expressions for $\langle u_i''(\boldsymbol{x},t)\Delta v_j(\boldsymbol{x},t|0)\rangle_\infty$ and $\langle u_i''(\boldsymbol{x},t)\Delta x_2(\boldsymbol{x},t|0)\rangle_\infty$ from (5.9), we obtain

$$\overline{u_i'v_j'}_{\infty} = \frac{\beta}{\beta+1}\langle u_i''u_j''\rangle_\infty - \delta_{j1}\frac{S\beta^2}{(\beta+1)^2}\langle u_i''u_2''\rangle_\infty. \tag{5.12}$$

5.2. *Ignoring the inertial acceleration term* $(\mathrm{D}/\mathrm{D}t)\overline{u_i''}$ *in the GLM approach*

For the simple mean shear defined in (5.4), and with $\alpha_{ij} = \alpha\delta_{ij}$ as in SDM, equation (4.5) reduces to

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{u_i''} = -\frac{\partial}{\partial x_j}\overline{v_j'u_i'}\langle\rho\rangle + \langle\rho\rangle\frac{\partial}{\partial x_j}\langle u_j'u_i'\rangle - \alpha\overline{u_i''}\langle\rho\rangle - S\delta_{i1}\overline{u_2''}\langle\rho\rangle. \tag{5.13}$$

Letting $t\to\infty$, and following the same procedure and assumptions made by Rogers *et al.* (1989), SDM ignore the contribution from the inertial acceleration term and write this equation as

$$O_{ij}\overline{u_i''}\langle\rho\rangle = -\overline{u_i'v_j'}\frac{\partial\langle\rho\rangle}{\partial x_j} \tag{5.14}$$

with

$$O_{ij} = \alpha\delta_{ij} + S\delta_{i1}\delta_{j2}. \tag{5.15}$$

That is, $\langle\rho\rangle\overline{u_i''}$ may be written in Boussinesq form as

$$\overline{u_i''}\langle\rho\rangle = -\epsilon_{ij}^{(fp)}\frac{\partial\langle\rho\rangle}{\partial x_j} \tag{5.16}$$

where

$$\epsilon_{ij}^{(fp)} = O_{im}^{-1}\overline{u_m'v_j'}. \tag{5.17}$$

Inverting the tensor $\boldsymbol{O}$ gives

$$O_{ij}^{-1} = \alpha^{-1}\delta_{ij} - \alpha^{-2}S\delta_{i1}\delta_{j2} \tag{5.18}$$

so that $\epsilon_{ij}^{(fp)}$ becomes

$$\epsilon_{ij}^{(fp)} = \alpha^{-1}\overline{u_i'v_j'} - \alpha^{-2}S\delta_{i1}\overline{u_2'v_j'}. \tag{5.19}$$

We would not expect the same expression for this coefficient as that given in (5.9) using the KM approach because (5.9) is based on an exponentially decaying correlation for the carrier flow along a particle trajectory which, as we shall see later, is not the form consistent with the SDM equation. There are however fundamental differences which do not depend upon the form of this carrier flow correlation, namely the values of $\langle u_i''(t)\Delta x_j(t)\rangle_\infty$ are in general fundamentally different from the values given by (5.19), indeed to such a degree that, as we shall later for a fluid point, the values of the normal streamwise components in a simple shear based on (5.19) are of opposite sign to those of $\langle u_i''(t)\Delta x_j(t)\rangle_\infty$.

5.3. *Evaluation for a Gaussian process*

The crucial point to make here is that setting the inertial acceleration term equal to zero in (4.5) for the mean drift velocity $\overline{\boldsymbol{u}''}$ is incompatible with a Gaussian process which encompasses the more general case of a uniform shear, where the elements of $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$ are constants independent of $\boldsymbol{x}$, the turbulence is homogeneous and stationary and $\langle \boldsymbol{u} \rangle$ is either constant or a uniform mean shear, so that

$$\langle u_i \rangle = S_{ij} x_j. \tag{5.20}$$

To show this we need to call on some basic results for Gaussian processes.

5.3.1. *Some basic properties*

To show that for a Gaussian process for $\boldsymbol{v}, \boldsymbol{x}, \boldsymbol{u}$, the inertial acceleration term cannot be ignored, we first need to establish some basic properties of this process (for more details see Swailes *et al.* 1995).

In this case the PDF (2.16) can be written as a classic Fokker–Planck equation

$$\frac{\partial \langle P \rangle}{\partial t} = \frac{\partial}{\partial p_i} \left\{ -A_{ij} p_j + \frac{\partial}{\partial p_k} B_{kj} \right\} \langle P \rangle \tag{5.21}$$

where

$$\boldsymbol{p} = \{v_1, v_2, v_3, u_1, u_2, u_3, x_1, x_2, x_3\}^T = \{\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}\}^T \tag{5.22}$$

and

$$\boldsymbol{A} = \begin{pmatrix} -\boldsymbol{\beta} & \boldsymbol{\beta} & \boldsymbol{0} \\ \boldsymbol{S} & -(\boldsymbol{S}+\boldsymbol{\alpha}) & \alpha \cdot \boldsymbol{S} + \boldsymbol{S}^2 \\ \boldsymbol{I} & \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}, \quad \boldsymbol{B} = \begin{pmatrix} \boldsymbol{0} & & \\ & \boldsymbol{C} & \\ & & \boldsymbol{0} \end{pmatrix} \tag{5.23}$$

$$C_{ij} = \int_0^\infty \langle f_i''(0) f_j''(s) \rangle \, \mathrm{d}s. \tag{5.24}$$

We consider the solution to this equation for a point source when all the particles are released into the flow at one point in phase space at some initial time which we will take to be $t = 0$. For convenience we shall consider $\langle P \rangle$ to be suitably normalized so that its integral over all particle velocities and fluid velocities and positions is unity. The solution for $\langle P \rangle$ can be found by taking the Fourier transformation of (5.21) with respect to $\tilde{p}$ which gives

$$\frac{\partial \tilde{P}}{\partial t} = \tilde{p}_i \left\{ A_{ij} \frac{\partial}{\partial \tilde{p}_j} - \tilde{p}_j B_{ji} \right\} \tilde{P} \tag{5.25}$$

where $\tilde{P}$ is the Fourier transform of $\langle P \rangle$ or the characteristic function

$$\tilde{P} = \langle \exp(\mathrm{i} \boldsymbol{p} \cdot \tilde{\boldsymbol{p}}) \rangle \tag{5.26}$$

which from (5.25) has a formal solution

$$\tilde{P} = \exp\{\mathrm{i} \tilde{\boldsymbol{p}} \cdot \hat{\boldsymbol{p}}\} \exp\left\{-\tfrac{1}{2} \tilde{\boldsymbol{p}} \cdot \Theta \cdot \tilde{\boldsymbol{p}}\right\} \tag{5.27}$$

of which $\hat{\boldsymbol{p}}$ is the time-dependent mean of $\boldsymbol{p}(t)$ in the absence of turbulence, i.e. the absence of white noise in the equation for $\boldsymbol{u}$ (equation (2.14)) The equation for $\hat{\boldsymbol{p}}$ is thus

$$\dot{\hat{\boldsymbol{p}}} = \boldsymbol{A} \cdot \hat{\boldsymbol{p}}. \tag{5.28}$$

Noting that, we can write

$$\hat{\boldsymbol{p}} = (\hat{\boldsymbol{v}}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{x}}) \tag{5.29}$$

where $\hat{\boldsymbol{v}}, \hat{\boldsymbol{u}}, \hat{\boldsymbol{x}}$ are time-dependent means of $\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}$ respectively in the absence of turbulence, $\boldsymbol{\Theta}$ is the matrix whose elements are the ensemble averages of covariance of $\boldsymbol{p}$ along all particle trajectories, i.e.

$$\begin{aligned}\boldsymbol{\Theta}(t) = \langle \boldsymbol{p}^* \boldsymbol{p}^*(t) \rangle &= \langle (\boldsymbol{p} - \hat{\boldsymbol{p}})(\boldsymbol{p} - \hat{\boldsymbol{p}}) \rangle \\ &= \begin{pmatrix} \langle \boldsymbol{v}^* \boldsymbol{v}^* \rangle & \langle \boldsymbol{v}^* \boldsymbol{u}^* \rangle & \langle \boldsymbol{v}^* \boldsymbol{x}^* \rangle \\ \langle \boldsymbol{u}^* \boldsymbol{v}^* \rangle & \langle \boldsymbol{u}^* \boldsymbol{u}^* \rangle & \langle \boldsymbol{u}^* \boldsymbol{x}^* \rangle \\ \langle \boldsymbol{x}^* \boldsymbol{v}^* \rangle & \langle \boldsymbol{x}^* \boldsymbol{u}^* \rangle & \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle \end{pmatrix}\end{aligned} \tag{5.30}$$

where $\boldsymbol{v}^* = \boldsymbol{v} - \hat{\boldsymbol{v}}$, $\boldsymbol{u}^* = \boldsymbol{u} - \hat{\boldsymbol{u}}$ and $\boldsymbol{x}^* = \boldsymbol{x} - \hat{\boldsymbol{x}}$.

$\boldsymbol{\Theta}$ is the solution of

$$\dot{\boldsymbol{\Theta}} = \boldsymbol{A} \cdot \boldsymbol{\Theta} + (\boldsymbol{A} \cdot \boldsymbol{\Theta})^T + 2\boldsymbol{B}. \tag{5.31}$$

The inverse Fourier transform of $\tilde{P}$ gives for $\langle P \rangle$

$$\langle P \rangle = (2\pi)^{-9/2} \det[\boldsymbol{\Theta}]^{-1/2} \exp\left[-\tfrac{1}{2} \boldsymbol{p}^{*T} \boldsymbol{\Theta}^{-1} \boldsymbol{p}^*\right]. \tag{5.32}$$

It also follows that the spatial mass concentration $\langle \rho \rangle$ is Gaussian since this represents the marginal distribution of $\langle P \rangle$. Indeed after some algebraic manipulation we obtain

$$\langle \rho \rangle = (2\pi)^{-3/2} \det[\langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle]^{-1/2} \exp\left[-\tfrac{1}{2} \boldsymbol{x}^{*T} \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1} \boldsymbol{x}^*\right] \tag{5.33}$$

with $\langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1} = \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1^T}$. We note for future reference that

$$\boldsymbol{x}^* \langle \rho \rangle = -\langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle \cdot \frac{\partial \langle \rho \rangle}{\partial \boldsymbol{x}^*}. \tag{5.34}$$

From (5.32) we also have for the particle density-weighted mean velocity and mean carrier flow velocity,

$$\bar{\boldsymbol{v}} = \hat{\boldsymbol{v}} + \langle \boldsymbol{v}^* \boldsymbol{x}^* \rangle \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1} \boldsymbol{x}^*, \tag{5.35}$$

$$\bar{\boldsymbol{u}} = \hat{\boldsymbol{u}} + \langle \boldsymbol{u}^* \boldsymbol{x}^* \rangle \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1} \boldsymbol{x}^*, \tag{5.36}$$

and for the covariances

$$\langle \boldsymbol{v}' \boldsymbol{v}' \rangle = \langle \boldsymbol{v}^* \boldsymbol{v}^* \rangle - \langle \boldsymbol{v}^* \boldsymbol{x}^* \rangle \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1} \langle \boldsymbol{x}^* \boldsymbol{v}^* \rangle, \tag{5.37}$$

$$\langle \boldsymbol{v}' \boldsymbol{u}' \rangle = \langle \boldsymbol{v}^* \boldsymbol{u}^* \rangle - \langle \boldsymbol{v}^* \boldsymbol{x}^* \rangle \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1} \langle \boldsymbol{x}^* \boldsymbol{u}^* \rangle. \tag{5.38}$$

5.3.2. *Evaluation of* $\langle \rho \rangle (\mathrm{D}/\mathrm{D}t) \overline{u_i''}$

We note that if we change to a frame of reference in which the variable $\boldsymbol{p}$ changes to $\boldsymbol{p}^*$, the equation of motion in these new variables and therefore in this new frame of reference remains unchanged provided that the white noise function in (2.14) is a function of time only. So the transport equation for $\langle P \rangle(\boldsymbol{v}^*, \boldsymbol{u}^*, \boldsymbol{x}^*, t)$ is the same as that for $\langle P \rangle(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t)$ in this new frame of reference. Similarly the transport equations for the density-weighted velocity averages associated with $\boldsymbol{v}^*$and $\boldsymbol{u}^*$ will be the same as those for $\boldsymbol{v}$ and $\boldsymbol{u}$. It is convenient therefore to consider the transport equations for these quantities in this new frame of reference since this eliminates any arbitrary dependence on initial conditions. The relationships that we develop for the transformed velocities $(\boldsymbol{v}^*, \boldsymbol{u}^*)$ for the Gaussian process will then be the same for the variables $\boldsymbol{v}$ and $\boldsymbol{u}$ in the original lab frame of reference. This will be equivalent to solving for the set of variables $(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t)$ with initial conditions $\hat{\boldsymbol{p}} = 0$.

Using therefore the Gaussian properties set out above and in particular those in (5.34)–(5.36) with $\hat{\boldsymbol{p}} = 0$, we evaluate the substantial derivative term in the transport equation (4.5) for the particle density-weighted fluid velocity $\overline{\boldsymbol{u}''}$ viewed by the particle and show that it is of the same order in the spatial concentration gradient as the other spatial gradient concentration terms. We have explicitly

$$\begin{aligned}\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{u_i''} &= \langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\bar{u}_i - \langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\langle u_i\rangle \\ &= \langle\rho\rangle\frac{\partial\bar{u}_i}{\partial t} + \langle\rho\rangle\bar{v}_j\frac{\partial\bar{u}_i}{\partial x_j} + S_{ik}\langle v_k x_j\rangle\frac{\partial\langle\rho\rangle}{\partial x_j}\end{aligned} \tag{5.39}$$

where we have used (5.34) to rewrite $\langle\rho\rangle\langle u_i\rangle$ in terms of the mean particle concentration gradient.

We now evaluate in turn the first two terms on the right-hand side of this equation for a Gaussian process.

5.3.3. *Evaluation of* $\langle\rho\rangle\partial\bar{u}_i/\partial t$

From (5.36) and using (5.34), we have

$$\begin{aligned}\langle\rho\rangle\frac{\partial\bar{u}_i}{\partial t} &= \langle\rho\rangle\frac{\partial}{\partial t}\left\{\langle u_i x_j\rangle\langle\boldsymbol{xx}\rangle^{-1}_{jk}x_k\right\} \\ &= -\left\{\frac{\partial\langle u_i x_j\rangle}{\partial t} - \langle u_i x_l\rangle\langle\boldsymbol{xx}\rangle^{-1}_{lk}\frac{\partial\langle x_k x_j\rangle}{\partial t}\right\}\frac{\partial\langle\rho\rangle}{\partial x_j} \\ &= -\left\{\langle\dot{u}_i x_j\rangle + \langle u_i v_j\rangle - \langle u_i x_l\rangle\langle\boldsymbol{xx}\rangle^{-1}_{lk}(\langle v_k x_j\rangle + \langle x_k v_j\rangle)\right\}\frac{\partial\langle\rho\rangle}{\partial x_j} \\ &= -\left\{\langle\dot{u}_i x_j\rangle + \langle u_i' v_j'\rangle - \langle u_i x_l\rangle\langle\boldsymbol{xx}\rangle^{-1}_{lk}\langle v_k x_j\rangle\right\}\frac{\partial\langle\rho\rangle}{\partial x_j}.\end{aligned} \tag{5.40}$$

5.3.4. *Evaluation of* $\langle\rho\rangle\bar{v}_j\partial\bar{u}_i/\partial x_j$

$$\begin{aligned}\langle\rho\rangle\bar{v}_j\frac{\partial\bar{u}_i}{\partial x_j} &= \langle v_j x_k\rangle\langle\boldsymbol{xx}\rangle^{-1}_{kl}x_l\langle\rho\rangle\langle u_i x_m\rangle\langle\boldsymbol{xx}\rangle^{-1}_{mn}\delta_{nj} \\ &= -\langle v_j x_k\rangle\langle\boldsymbol{xx}\rangle^{-1}_{kl}\langle u_i x_m\rangle\langle x_l x_n\rangle\frac{\partial\langle\rho\rangle}{\partial x_n}\langle\boldsymbol{xx}\rangle^{-1}_{mj} \\ &= -\langle v_j x_k\rangle\langle\boldsymbol{xx}\rangle^{-1}_{mj}\langle x_m u_i\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}.\end{aligned} \tag{5.41}$$

So after combining (5.40) and (5.41) we have

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\bar{u}_i = -\{\langle\dot{u}_i x_j\rangle + \langle u_i' v_j'\rangle\}\frac{\partial\langle\rho\rangle}{\partial x_j} \tag{5.42}$$

and in turn the result

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{u_i''} = -\{\langle\dot{u}_i x_j\rangle + \langle u_i' v_j'\rangle - S_{ik}\langle v_k x_j\rangle\}\frac{\partial\langle\rho\rangle}{\partial x_j}. \tag{5.43}$$

5.3.5. *Evaluation of* $\langle\rho\boldsymbol{u}''\rangle$

Using the Gaussian expression for $\langle\rho\rangle(\mathrm{D}/\mathrm{D}t)\bar{u}_i$ in (5.42), we derive an expression for $\langle\rho\boldsymbol{u}''\rangle$ starting from the momentum equation for $\bar{\boldsymbol{u}}$, namely equation (4.3), recognizing that when the turbulence is homogeneous $f_i(\boldsymbol{x})=0$, so we have

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\bar{u}_i = \left\{\alpha_{ij}(\langle u_j\rangle - \bar{u}_j) + (\bar{v}_j - \bar{u}_j)\frac{\partial\langle u_i\rangle}{\partial x_j}\right\}\langle\rho\rangle - \langle u_i' v_j'\rangle\frac{\partial\langle\rho\rangle}{\partial x_j}. \tag{5.44}$$

Substituting the expression for $\langle\rho\rangle(\mathrm{D}/\mathrm{D}t)\bar{u}_i$ given in (5.42) and using (2.14) we obtain

$$\alpha_{ij}\langle u''_j x_k\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}-\frac{\partial\langle u_i\rangle}{\partial x_j}\{\langle v_j x_k\rangle-\langle u_j x_k\rangle\}\frac{\partial\langle\rho\rangle}{\partial x_k}-\langle f''_i x_k\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}$$
$$=\left\{-\alpha_{ij}\overline{u''}_j\langle\rho\rangle+\frac{\partial\langle u_i\rangle}{\partial x_j}(\bar{v}_j-\bar{u}_j)\langle\rho\rangle\right\}. \tag{5.45}$$

This equation is satisfied if the following relationships hold:

$$\langle\rho\rangle\bar{v}_j=-\langle v_j x_k(t)\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}, \tag{5.46}$$

$$\langle\rho\rangle\bar{u}_j=-\langle u_j x_k(t)\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}, \tag{5.47}$$

$$\langle\rho\rangle\overline{u''_i}=-\langle u''_j x_k(t)\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}, \tag{5.48}$$

$$\langle f''_i x_k(t)\rangle=0. \tag{5.49}$$

The relationships (5.46), (5.47) are valid for the Gaussian distribution given in (5.32) which is also true for (5.48) since we have from (5.47) and (2.6),

$$\langle\rho\rangle\overline{u''_j}+\langle\rho\rangle\langle u_j\rangle=-\langle u_j x_k(t)\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}, \tag{5.50}$$

i.e.

$$\langle\rho\rangle\overline{u''_j}+\langle\rho\rangle S_{ij}x_j=-\langle u''_j x_k\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}-S_{jl}\langle x_l x_k\rangle\frac{\partial\langle\rho\rangle}{\partial x_k}. \tag{5.51}$$

Using (5.34) we have

$$\langle\rho\rangle\overline{u''_j}=-\langle u''_j x_k\rangle\frac{\partial\langle\rho\rangle}{\partial x_k} \tag{5.52}$$

which is consistent with (5.48). The last relationship (5.49), is true for a white noise function.

5.4. *Summary and conclusions of analysis*

The relationships for the mean flow velocity encountered by the particle $\langle\rho\rangle\overline{u''_j}$ etc. above are properties of the Gaussian distribution that is a solution of the transport equations in homogeneous turbulence with or without a mean shear (see (5.32)), results we could have deduced from the form of $\langle P\rangle$ in (5.32) at the outset. The analysis we have carried out in § 5.3.5 merely confirms it. The real purpose of the analysis has been to show that these relationships are consistent with the form for $\mathrm{D}\overline{\boldsymbol{u}''}/\mathrm{D}t$ we have obtained from the Gaussian distribution and the transport equation for $\bar{u}_i$ and in particular that $\mathrm{D}\overline{\boldsymbol{u}}/\mathrm{D}t$ is proportional to the local particle concentration gradient. Furthermore the form for $\langle\rho\rangle\overline{u''_i}$ is consistent with the form given by KM, that is integrating (2.9) over all velocities, and noting that in homogeneous turbulence the second term on the right-hand side of (2.9) is zero, we arrive at the form in (5.52).

So in summary, the discrepancy between the forms of the fluid-particle diffusion coefficient based on the two PDF approaches for dispersion in a uniform shear arises from an incorrect modelling assumption in the application of the GLM transport equation for the mean flow velocity encountered by the particle in the long-term limit, namely that the inertial acceleration term $\mathrm{D}\overline{\boldsymbol{u}''}/\mathrm{D}t$ may be set to zero, thus leading to a set of algebraic expressions for the fluid-particle diffusion coefficients. The diffusion process is Gaussian in the uniform shear case which means that whilst this inertial term does tend to zero, it tends to zero at the same rate as the other terms in the equation since they are all proportional to the particle concentration gradient. So setting this term to zero and retaining the other terms in the equation is inconsistent. In this analysis we evaluated the value of this term for a Gaussian process and then included it in the transport equation for the mean flow velocity (encountered by the particle) and showed that the resulting value for $\langle\rho\rangle\overline{u''_j}$ is the same as that given by the KM approach. We shall see later that in the case of passive scalar dispersion, Rogers *et al.* (1989) assume that the equivalent inertial term is proportional to the mean scalar quantity rather than the mean scalar gradient as for Gaussian process: the end result is the same as neglecting the inertial term. We will consider the magnitude of the discrepancy graphically in the next section when we present exact solutions for the particle and carrier flow (seen by the particle) for the simple shear flow case.

6. Explicit solutions for the GLM approach for dispersion in a simple shear

In this section we present analytic expressions for the long-term (equilibrium) values for the statistical ensemble averages of the Gaussian process associated with dispersion in a simple shear. In particular we will evaluate the phase-space diffusion coefficients $\langle u''_i(t)\Delta x_j(t)\rangle$ and $\langle u''_i(t)\Delta v_j(t)\rangle$ for the simple case when α in the Pope model for the continuous phase is independent of the local shear. More complicated functions for α could have been chosen of course but in this case, relatively simple algebraic expressions can be obtained for the long-term ensemble averages as functions of the strain rate S and the inverse particle response time β; these algebraic expressions contain some important properties we wish to illustrate and discuss. In addition to the phase-space diffusion coefficients, we have also obtained algebraic expressions for the long-term value of the second moments associated with the processes $[\boldsymbol{v}'', \boldsymbol{u}'']$ and $[\boldsymbol{v}'', \boldsymbol{x}]$ where $\boldsymbol{v}''$ is the particle velocity relative the local mean carrier flow velocity $\langle\boldsymbol{u}\rangle$ at $\boldsymbol{x}(t)$. We also consider the way in which these moments reach their long-term equilibrium values by numerically solving the moment equations themselves which are a set of coupled linear ODEs.† These moments are sufficient to determine all the second moments associated with the process $[\boldsymbol{v}, \boldsymbol{x}, \boldsymbol{u}]$ which in turn enables us to evaluate precisely the way the concentration of particles evolves with time for particles initiating from the centre of the mean shear.

Important additions to this process not considered previously are the spatial and time dependence of the mean and covariance of the carrier flow velocity field encountered by the dispersing particles. This of course is the extra information we can obtain using the GLM approach compared to the KM approach. We will also consider this along with the temporal and spatial dependence of the mean particle velocity field at the end of the section.

6.1. *Analytic expressions for the long-term phase-space diffusion coefficients and fluid-particle covariances*

To illustrate the similarity between the two PDF approaches, we have evaluated the phase-space diffusion coefficients in the GLM approach using the method described in § 5.1 for the KM approach. To do this we first need to evaluate the autocorrelation function $\langle u''_i(0)u''_j(t)\rangle$ associated with the process defined by the SDM equation (2.14). Thus we consider two functions $F_1(t)$ and $F_2(t)$ which are linearly related

† The equations could have been solved analytically but it was simpler and more efficent to solve them numerically by standard methods.

to some random stationary driving force $f(t)$ via response functions $G_1(t)$ and $G_2(t)$ respectively, i.e.

$$F_i(t) = \int_0^t G_i(t-s) f(s)\,\mathrm{d}s, \quad i = 1, 2, \tag{6.1}$$

Thus we have

$$\langle F_1(t_1) F_2(t_2)\rangle = \int_0^{t_1} \mathrm{d}s_1 \int_0^{t_2} \mathrm{d}s_2 G_1(t_1 - s_1) G_2(t_2 - s_2) R(s_2 - s_1) \tag{6.2}$$

with

$$R(s_2 - s_1) = R(s_1 - s_2) = \langle f(s_1) f(ts_2)\rangle. \tag{6.3}$$

Introducing the delta-correlated approximation $R(s_2 - s_1) \approx C\delta(s_2 - s_1)$ appropriate for a white noise function $f(s)$ gives for $t_2 > t_1 \to \infty$

$$\langle F_1(t_1) F_2(t_2)\rangle = C \int_0^\infty G_1(s) G_2(t_2 - t_1 + s)\,\mathrm{d}s.$$

In the case of $F_1(t_1) = u_i''(t_1)$, $F_2(t_1) = u_j''(t_2)$ we have

$$\langle u_i''(t_1) u_j''(t_2)\rangle = C \int_0^\infty \mathrm{d}s G_{ki}^{u''}(s) G_{kj}^{u''}(t_2 - t_1 + s), \quad t_2 > t_1,$$

and by implication for $t_2 < t_1$

$$\left\langle u_j''(t_2) u_i''(t_1)\right\rangle = C \int_0^\infty \mathrm{d}s G_{kj}^{u''}(s) G_{ki}^{u''}(t_1 - t_2 + s), \quad t_2 < t_1.$$

Using the response functions for $G_{ij}^{u''}(t)$ given in the Appendix (see equation (A 2)) gives for the case $\langle u_i''(t_1) u_i''(t_2)\rangle$

$$\left.\begin{aligned} \langle u_1''(0) u_1''(\tau)\rangle &= \langle u_2''^2\rangle \mathrm{e}^{-|\tau|} \left\{1 + \tfrac{1}{2} S^2 (1 + |\tau|)\right\}, \\ \langle u_2''(0) u_2''(\tau)\rangle &= \langle u_2''^2\rangle \mathrm{e}^{-|\tau|}. \end{aligned}\right\} \tag{6.4}$$

The shape and dependence of the autocorrelation coefficient upon τ and S are shown in figure 1. For the cross-correlation $\langle u_1''(0) u_2''(\tau)\rangle$, substituting the appropriate forms for $G_{ki}^{u''}(s)$ gives the result

$$\left.\begin{aligned} \langle u_1''(0) u_2''(\tau)\rangle &= -\tfrac{1}{2}\langle u_2''^2\rangle S \mathrm{e}^{-\tau}, \quad \tau \geqslant 0, \\ &= -\tfrac{1}{2}\langle u_2''^2\rangle S \mathrm{e}^{\tau}(1 - 2\tau), \quad \tau \leqslant 0, \end{aligned}\right\} \tag{6.5}$$

and this is illustrated graphically in figure 2. We note first that in this case, the process is not symmetric in time, i.e.

$$\langle u_1''(0) u_2''(\tau)\rangle \neq \langle u_1''(0) u_2''(-\tau)\rangle,$$

and secondly the maximum correlation does not occur when $\tau = 0$!

Using these functional forms for the autocorrelation function together with the response functions $\boldsymbol{G}^x(t)$ for displacements in the shear given in (5.6) and (5.7), the long-term phase-space dispersion coefficients have been evaluate:

$$\langle u_i''(t) x_j(t)\rangle_{t\to\infty} = \langle u_2''^2\rangle \alpha^{-1} \begin{bmatrix} \dfrac{\beta}{\beta+1} - S^2 \dfrac{\beta(3\beta^2 + 4\beta - 3)}{2(\beta+1)^3} & -S\dfrac{\beta(3\beta+5)}{2(\beta+1)^2} \\ S\dfrac{\beta(\beta-1)}{2(\beta+1)^2} & \dfrac{\beta}{\beta+1} \end{bmatrix} \tag{6.6}$$

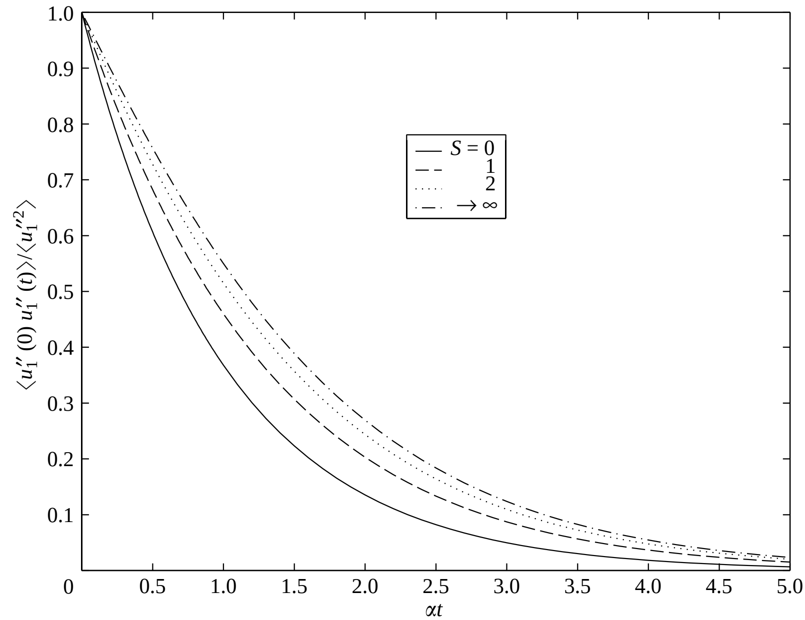

FIGURE 1. Autocorrelation function $\langle u_1''(0)u_1''(t)\rangle$ based on SDM equation (2.14).

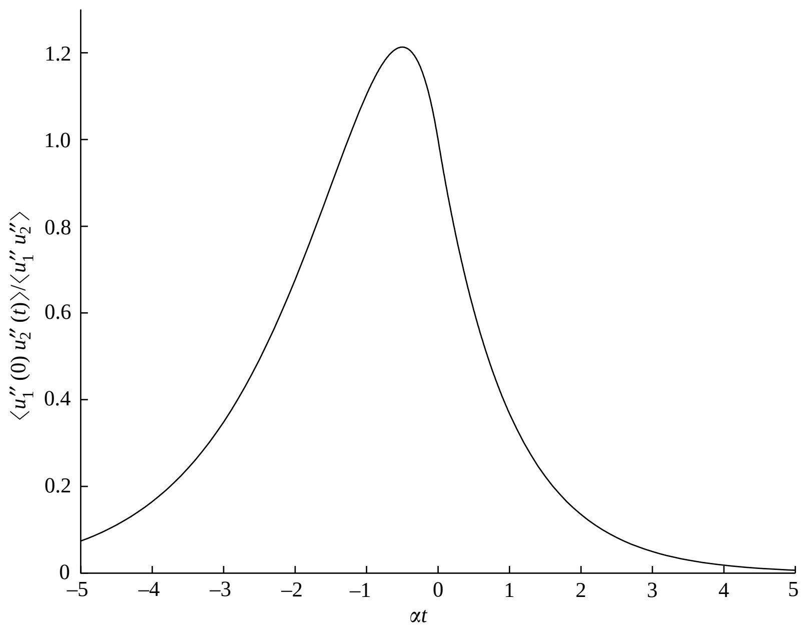

FIGURE 2. Autocorrelation function $\langle u_1''(0)u_2''(t)\rangle$ based on SDM equation (2.14).

and

$$\langle u_i''(t)v_j(t)\rangle_{t\to\infty} = \left\langle u_2''^2\right\rangle \begin{bmatrix} \dfrac{\beta}{\beta+1} - S^2\dfrac{\beta(\beta^2+2\beta-1)}{(\beta+1)^3} & -S\dfrac{\beta(\beta+3)}{2(\beta+1)^2} \\ S\dfrac{\beta(\beta-1)}{2(\beta+1)^2} & \dfrac{\beta}{\beta+1} \end{bmatrix} \tag{6.7}$$

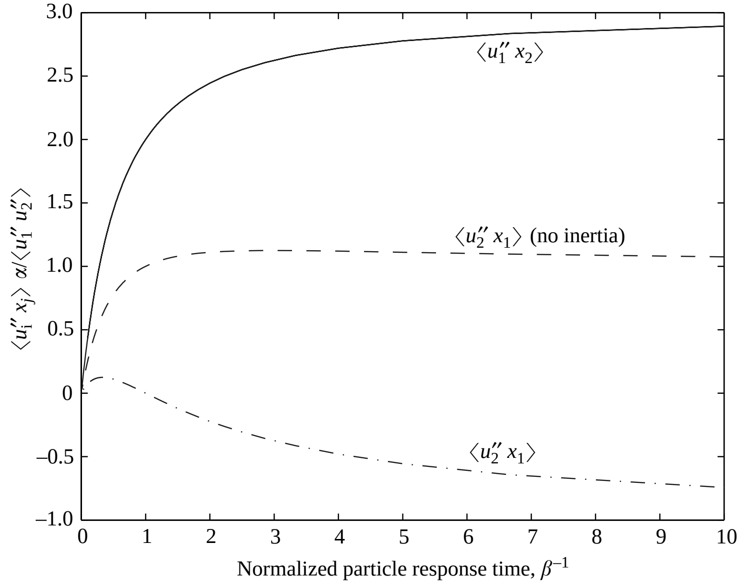

FIGURE 3. Long-time off-diagonal fluid-particle spatial diffusion coefficients $\langle u_i'' x_j \rangle$, $i \neq j$. Note that the values of the $i=1$, $j=2$ components with and without inertia are the same.

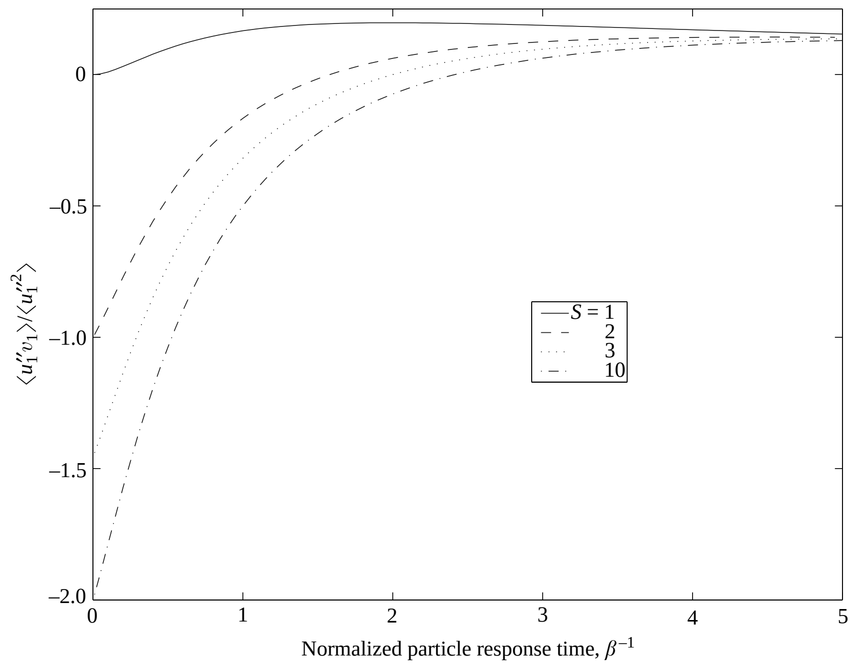

FIGURE 4. Long-time streamwise fluid-particle velocity diffusion coefficient $\langle u_1'' v_1 \rangle$.

and these are illustrated graphically in figures 3–5. To check that the expressions given in (6.6) and (6.7) are correct, they were also obtained from the moment equations derived by appropriately integrating the PDF equation over all $\boldsymbol{v}$, $\boldsymbol{x}$, $\boldsymbol{u}$. This alternative method avoids explicit knowledge of $\langle u_i''(0) u_j''(t) \rangle$ and the response functions $\boldsymbol{G}^x(t)$.

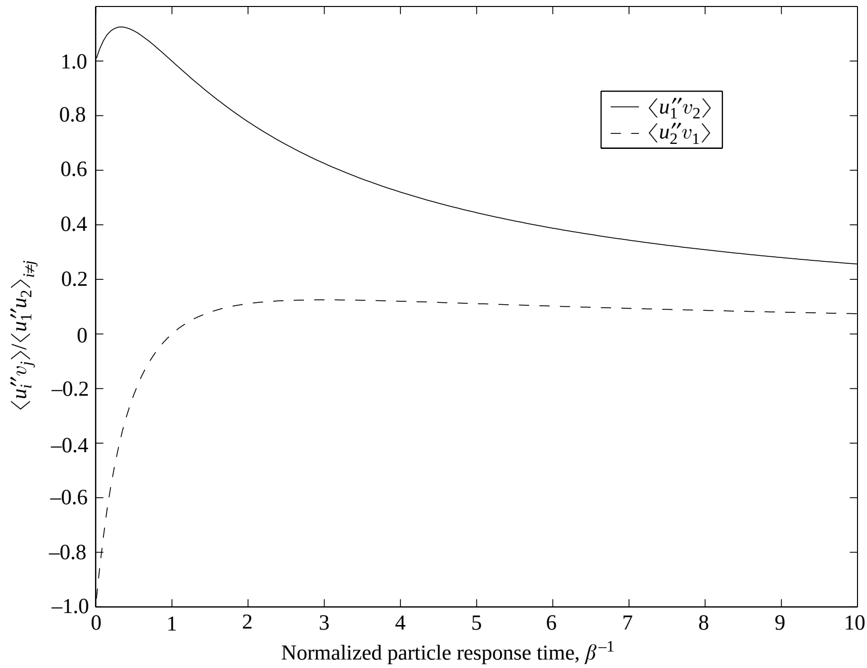

FIGURE 5. Long-time off-diagonal fluid-particle velocity diffusion coefficients $\langle u_i''v_j\rangle, i \neq j$.

We recall that each diffusion coefficient has both a homogeneous component and a deviatoric component. Referring to (5.9) as a typical example where the homogeneous and deviatoric components can easily be identified, we note that the homogeneous component is always positive in relation to the corresponding fluid velocity covariances, e.g. $\langle u_1''(t)x_1(t)\rangle^{(0)}$ is always positive because $\langle u_1''^2\rangle$ is positive; the streamwise normal deviatoric components $\langle u_1''x_1\rangle, \langle u_1''v_1\rangle$ are always negative because $\langle u_1''u_2''\rangle$ is always negative whilst the cross-diagonal deviatoric components of $\langle u_2''x_1\rangle, \langle u_2''v_1\rangle$ are always positive because of the action of the shear on the particle motion. The other two deviatoric components are zero, i.e. the expressions given for $\langle u_1''x_2\rangle, \langle u_1''v_2\rangle$ in (6.6) and (6.7) are the homogeneous components. Thus because the total contribution of both the homogeneous and deviatoric components are additive, the phase-space diffusion coefficients in the cases where the deviatoric components are non-zero can be either positive or negative depending on the dependence of the homogeneous/deviatoric components upon the particle inertia β and strain rate S. In most cases increasing both β and S increases the absolute value of the diffusion coefficient. As an illustration see also figure 6 for the dependence on β^{-1} of both the homogeneous and deviatoric long-time components of $\langle u_1''x_1\rangle$ which is consistent with this pattern of behaviour. Note that the deviatoric component eventually obtains a very small positive value before finally decaying away to zero with increasing β^{-1}; hence also a similar behaviour for $\langle u_1''x_1\rangle$ shown in figure 7.

For the case of the fluid-particle spatial diffusion coefficients we have also shown the result of neglecting the inertial acceleration term in (5.13). The algebraic expressions for the fluid-particle spatial diffusion coefficient are obtained by substituting the

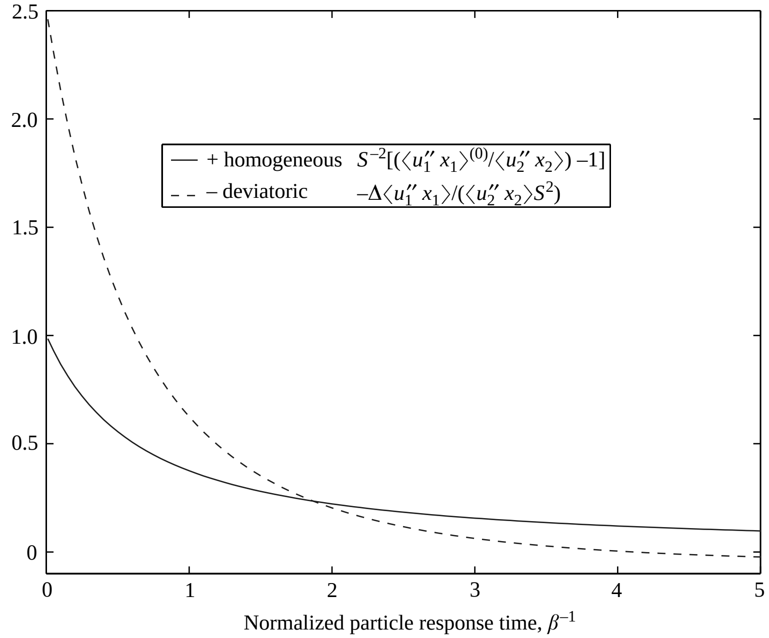

FIGURE 6. Equilibrium homogeneous and deviatoric components of the streamwise fluid-particle spatial diffusion coefficient $\langle u_1''x_1\rangle$.

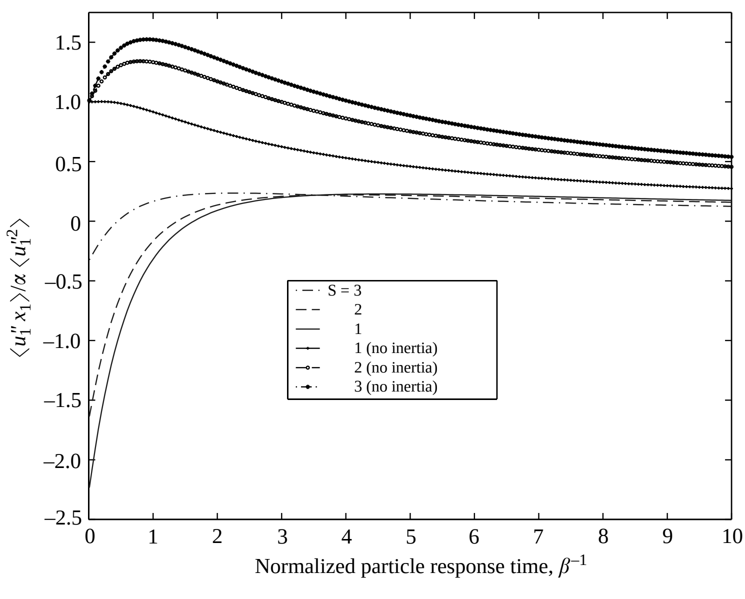

FIGURE 7. Long-time streamwise fluid-particle spatial diffusion coefficient $\langle u_1''x_1\rangle$.

long-term values for $\langle u_i'v_j'\rangle = \langle u_i''v_j''\rangle_\infty$ given in (6.8) into (5.19) which gives

$$\epsilon_{ij}^{(fp)} = \langle u_2''\rangle\alpha^{-1}\begin{bmatrix} \dfrac{\beta}{\beta+1} + S^2\beta\dfrac{\beta^2+5\beta+8}{2(\beta+1)^3} & -S\dfrac{\beta(3\beta+5)}{2(\beta+1)^2} \\ -S\dfrac{\beta(\beta+3)}{2(\beta+1)^2} & \dfrac{\beta}{\beta+1} \end{bmatrix}.$$

Their functional dependence is shown alongside the values of $\langle u_i'' x_j \rangle$ in figures 3 and 7. The differences are profound. Unlike $\langle u_1'' x_1 \rangle$ the corresponding value of $\epsilon_{ij}^{(fp)}$ without inertia is always positive. The difference is most striking for the case when $\beta^{-1} = 0$, that is for the fluid point spatial diffusion coefficient. This needs more careful consideration and we shall return to it at a later stage in § 6.4 when we consider the precise way in which the particles diffuse in the shear when these spatial diffusion coefficients are negative. Note also that the fluid-particle velocity diffusion coefficients exhibit similar properties, yet the velocity distribution is always realizable. In the end it is a matter of how we choose to describe the diffusion process. Note that in the case of $\langle u_1'' x_2 \rangle$ and $\langle u_1'' v_2 \rangle$ the two expressions with/without the inertial acceleration term agree, but we observe that in these cases the deviatoric components are zero, and it is through the existence of the deviatoric components that the fundamental differences between the methods of calculation occurs.

To complete the picture we also report the values of the fluid-particle velocity co-variances $\langle u_i' v_j' \rangle$ which in the long-term are the same as $\langle u_i'' v_j'' \rangle$:

$$\langle u_i'(t) v_j'(t) \rangle_{t\to\infty} = \langle u_2''^2 \rangle \begin{bmatrix} \dfrac{\beta}{\beta+1} + S^2 \dfrac{\beta(\beta^2+4\beta+7)}{(\beta+1)^3} & -S\dfrac{\beta(\beta+3)}{2(\beta+1)^2} \\ -S\dfrac{\beta(\beta+3)}{2(\beta+1)^2} & \dfrac{\beta}{\beta+1} \end{bmatrix}. \tag{6.8}$$

These expressions have been obtained using (4.2) for the KM approach and appropriate for a Gaussian process. They can also be obtained using the transport equation (4.6) for $\langle u_i' v_j' \rangle$ and ignoring the inertial acceleration term which in this case is a valid procedure as $t \to \infty$. Note that for this model $\langle u_1' v_2' \rangle = \langle u_2' v_1' \rangle$ which is not a general result.

6.2. *Analytic expressions for the long-time particle velocity covariances and spatial diffusion coefficients*

We give analytic expressions for the longer-term (equilibrium) ensemble averages $\langle v_i'' v_j'' \rangle_\infty$ and $\langle v_i'' x_j \rangle_\infty$ which determine the velocity and spatial distribution of the particles, in the long-term both of which are Gaussian. As before both sets of moments have both homogeneous and deviatoric components and it is interesting to consider the dependence of these quantities upon the particle response time. In these particular cases we have obtained the expressions by solving the appropriate set of coupled moment equations obtained by multiplying the PDF equation by $\langle v_i'' v_j'' \rangle$ or $\langle v_i'' x_j \rangle$ as required and integrating over all particle $\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}$ etc.

6.2.1. *Particle velocity covariances/kinetic (Reynolds) stresses*

The equilibrium particle velocity covariance matrix is given by

$$\frac{\langle v_i'' v_j'' \rangle_\infty}{\langle u_2''^2 \rangle} = \begin{bmatrix} \dfrac{\beta}{\beta+1} + S^2 \dfrac{(\beta^4+5\beta^3+12\beta^2+5\beta+1)}{2\beta(\beta+1)^3} & -S\dfrac{(\beta^2+4\beta+1)}{2(\beta+1)^2} \\ -S\dfrac{(\beta^2+4\beta+1)}{2(\beta+1)^2} & \dfrac{\beta}{\beta+1} \end{bmatrix} \tag{6.9}$$

and the normal streamwise and off-diagonal components (shear stresses) are shown graphically in figure 8. We recall from the previous analysis of Reeks (1993) for dispersion in a simple shear based on the transport equations for the particle kinetic/Reynolds stresses using the KM approach, that the deviatoric particle shear

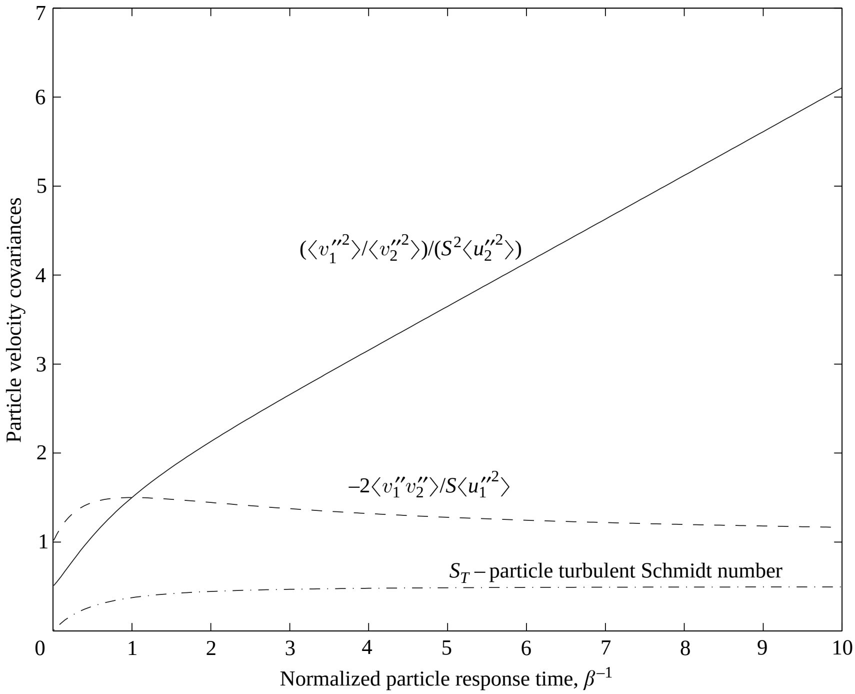

FIGURE 8. Long-time particle velocity covariances (particle Reynolds stresses) $\langle v_i''v_j''\rangle$ and particle Schmidt number as a function of the particle response time β^{-1}. The strain rate S is normalized on α^{-1}, the integral timescale of the carrier flow velocity in the cross-streamwise $i = 2$ direction.

stresses $\Delta \langle v_1''v_2''\rangle_\infty$ can be written as

$$\Delta \langle v_1''v_2''\rangle_\infty = \tfrac{1}{2}\Delta \langle u_2''v_1\rangle_\infty - S_p\nu_p \tag{6.10}$$

where S_p is the mean strain rate of the dispersed particle phase and ν_p the kinematic viscosity of the dispersed phase, given by

$$\nu_p = \tfrac{1}{2}\epsilon_{22}^0 \tag{6.11}$$

with ϵ_{22}^0 denoting the long-time diffusion coefficient in the cross-streamwise direction which is unaffected by the shear, i.e. it is based on the form for homogeneous flow. In this model $\epsilon_{22}^0 = \langle u_2''^2\rangle\alpha^{-1}$. Of course S_p is the same here as S but S_p was used in Reeks (1993) to distinguish the contribution from the shearing of the particle flow from that of the underlying carrier flow. The S_p term is a viscous term (not of course experienced by an individual particle) as distinct from the deviatoric component of the velocity dispersion coefficient $\langle u_2''v_1\rangle_\infty$ dependent on S and arising from the influence of the shearing of the carrier phase upon the motion of the particle. The deviatoric component of $\langle v_1''v_2''\rangle_\infty$ must have the property that it contracts to zero as the particle response time $\beta^{-1} \to 0$ so that

$$\Delta\langle v_1''v_2''\rangle_\infty \to -\tfrac{1}{2}(S_p - S)\langle u_2''^2\rangle \tag{6.12}$$

where both S_p and S are normalized on the Lagrangian integral timescale of the carrier flow motion in the x_2-direction. In the case considered here this timescale is

α^{-1}. For the SDM model we have in general

$$\frac{\Delta\langle v_1''v_2''\rangle_\infty}{\langle u_2''^2\rangle} = \frac{\beta^2}{2(\beta+1)^2}S - \frac{1}{2}S_p$$
$$= -S_T S \;\text{ with } S = S_p$$

where S_T represents the turbulent Schmidt number of the dispersed phase and is identical to the form given in equation (49) of Reeks (1993), namely

$$S_T = \frac{\beta + \frac{1}{2}}{(\beta+1)^2}. \tag{6.13}$$

The reason for the identity is because both expressions are based on an exponentially decaying correlation for the carrier flow velocity fluctuations along a particle trajectory, i.e. $\langle u_2(t)u_1(s)\rangle$ $s \leqslant t$ (see (6.5)).

The streamwise particle turbulent kinetic energy $\langle v_1''^2\rangle$ is related to the particle Reynolds shear stresses and the particle phase-space dispersion coefficients by

$$\langle v_1''^2\rangle = -\beta^{-1}S_p\langle v_1''v_2''\rangle + \langle u_1''v_1''\rangle. \tag{6.14}$$

From figure 8 and the expression for the Reynolds shear stresses (6.9) it is clear that the ratio $-\langle v_1''v_2''\rangle/2S\langle u_2''\rangle$ is not particularly sensitive to the particle response time, being unity when the response time is zero and also when the response time $\to \infty$, reaching a maximum of 1.5 for $\beta^{-1} = 0.5$. The consequence is that the contribution of the particle Reynolds stresses to the particle normal stresses in (6.14) increases as $\frac{1}{2}S^2\beta^{-1}$ and dominates the contribution from the particle-fluid covariances which tends to zero as β for $\beta^{-1} \to \infty$. That is as $\beta^{-1} \to \infty$, $\langle v_1''^2\rangle/\langle u_2''\rangle \to \frac{1}{2}S^2\beta^{-1}$ which is confirmed by the form for $\langle v_1''^2\rangle$ in figure 8.

6.2.2. *Particle spatial diffusion coefficients* $\langle v_i''x_j\rangle$

The unique feature of this linear system is that irrespective of the particle acceleration term $\mathrm{D}\overline{\boldsymbol{v}}/\mathrm{D}t$ (the inertial acceleration term), the spatial concentration can be represented by a convection diffusion equation in which the components of the particle flux $\boldsymbol{j}$ are given by

$$j_i = \langle u_i\rangle\langle\rho\rangle - \langle v_i''(t)x_j(t)\rangle\frac{\partial\langle\rho\rangle}{\partial x_j}. \tag{6.15}$$

The long-term (steady-state) forms of the particle spatial diffusion coefficients $\langle v_i''(t)x_j(t)\rangle$ are probably the most interesting because, like the fluid-particle diffusion coefficients, the influence of the inertial acceleration term, depending on the shear and the particle response time, can give them negative values. As with the particle Reynolds stresses, the long-term particle diffusion coefficients were evaluated by multiplying the PDF equation for $P(\boldsymbol{v}'', \boldsymbol{u}, \boldsymbol{x})$ by $\langle v_i''x_j\rangle$, integrating over all $\boldsymbol{v}'', \boldsymbol{u}, \boldsymbol{x}$ and setting $\partial/\partial t = 0$. The results for the long-term diffusion coefficients $\langle v_i''x_j\rangle_\infty$ are

$$\frac{\langle v_i''x_j\rangle_\infty}{\langle u_2''^2\rangle\alpha^{-1}} = \begin{bmatrix} 1 - S^2\dfrac{(3\beta^5+7\beta^4+4\beta^3+4\beta^2+7\beta+3)}{2\beta^2(\beta+1)^3} & -S\dfrac{(3\beta^3+8\beta^2+8\beta+3)}{\beta(\beta+1)^2} \\ S\dfrac{(\beta^3+1)}{\beta(\beta+1)^2} & 1 \end{bmatrix}. \tag{6.16}$$

The dependence of these coefficients on the particle response time is illustrated graphically in figure 9 from which we note that the cross-diagonal components are

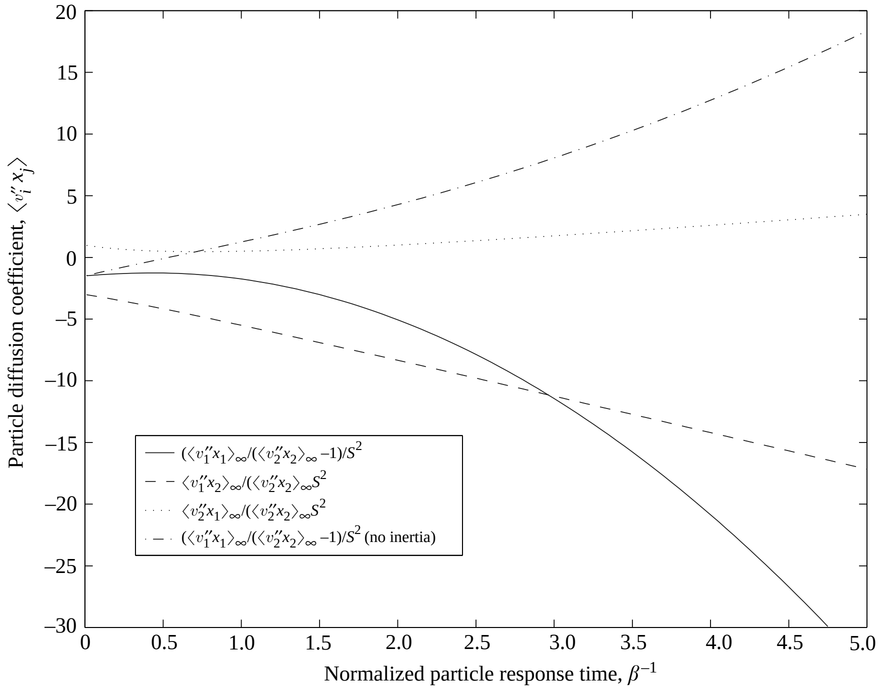

FIGURE 9. Long-time particle diffusion coefficients $\langle v_i'' x_j \rangle$ for the particle flux $\langle \rho v_i'' \rangle$.

of opposite sign and that the normal streamwise component is such that

$$\frac{\langle v_1'' x_1 \rangle_\infty}{\langle u_2''^2 \rangle \alpha^{-1}} \lesssim 1 - 1.257 S^2. \tag{6.17}$$

So the normal streamwise diffusion coefficient is $\leqslant 0$ irrespective of the value of particle response time, if $S \geqslant 0.8920$. In the case of the fluid point (the Pope model) this diffusion coefficient $\leqslant 0$ for $S \geqslant \sqrt{2/3}$. So both $\langle v_1'' x_1 \rangle_\infty$ and $\langle u_1'' x_1 \rangle_\infty$ share this negativity property, which is not surprising of course because they share the same origin. We shall discuss this property and its relevance to diffusion in more detail in the next section. Suffice it to say here, that the origin is linked to the influence of the shear itself and to the creation of positive Reynolds shear stresses both for the carrier flow and the dispersed phase. It is interesting to compare the values of the particle diffusion coefficients $\langle v_1'' x_1 \rangle_\infty$ with those obtained by neglecting the inertial acceleration term in the particle momentum equation, namely

$$D_{11} = \beta^{-1} \langle v_1''^2 \rangle_\infty + \langle u_1'' x_1 \rangle_\infty. \tag{6.18}$$

This is also shown in figure 9. The comparison is with the equivalent forms for the spatial fluid-particle diffusion coefficient under the same circumstances (see figure 7): however whereas the fluid-particle diffusion coefficient without the influence of inertia, is always positive, this is not the case for the equivalent particle diffusion coefficient since it contracts to the correct value for the carrier flow diffusion coefficient for $\beta^{-1} = 0$, though it is, in fact, positive for a significant range, namely for $\beta^{-1} > 0.53$.

6.3. *Evolution of the ensemble averages*

We consider here how the global averages associated with the dispersion process $[\boldsymbol{v}, \boldsymbol{x}]$ vary with time both in the short term and in the long term. In particular we consider

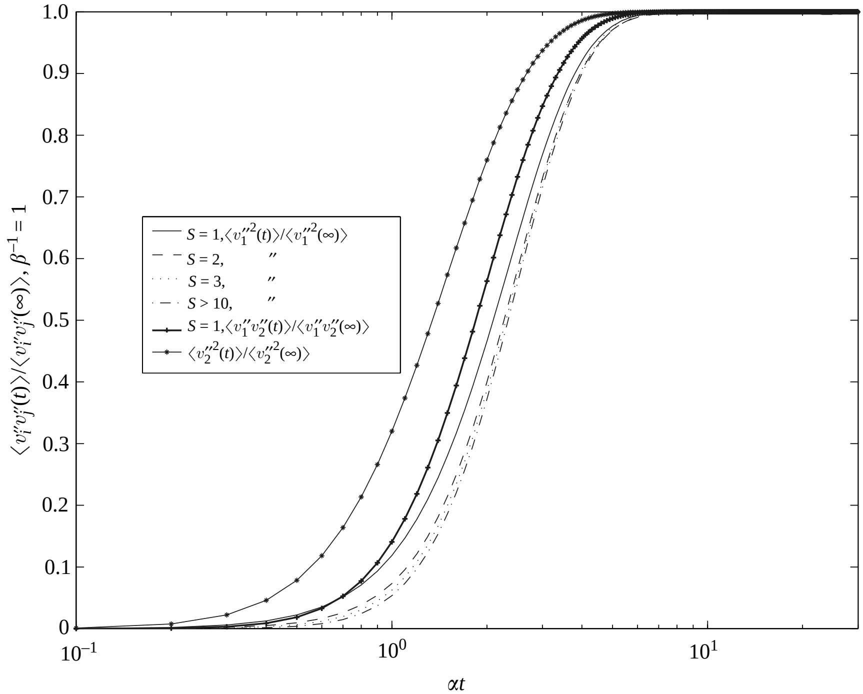

FIGURE 10. Time dependence of particle velocity covariances $\langle v_i''v_j''\rangle$ for $\beta^{-1} = 1$, and a range of values of S.

the role of the integral timescales of the turbulence $\sim\alpha^{-1}$ and the particle response time β^{-1} and also the role of the strain rate S. In the case we are considering here, we have normalized both β and S on α, so we only need to consider the dependence of the timescales on β and S. The particle velocity and carrier flow velocity encountered by the particle evolve from a prescribed set of initial conditions. In this particular case, the particles are introduced at the centre of the shear with a velocity of zero, which is the same as the carrier flow velocity that they encounter at that instance. In practice we could introduce particles with zero velocity but consider only those particles for which the carrier flow velocity encountered is zero or at least sufficiently close to zero. The fact that we introduce particles at the centre of the shear rather than anywhere else is a matter of convenience: we could have chosen any point in the shear and then transformed to a frame of reference moving with velocity equal to that of the mean shear at that point and the results would be the same.

There are essentially two processes evolving with different timescales. The first is the carrier flow encountered by the particle itself which evolves towards the equilibrium distribution of the whole carrier flow as the particle mixes with the flow. In this particular SDM model the scale of this carrier flow mixing is $\sim\alpha^{-1}$ irrespective of the particle response time (generally this would not be the case). The second process is the way the particle responds to the carrier flow, to both the shear and the turbulence, which will be dominated by the response time β^{-1}.

Figures 10 and 11 for the particle velocity covariances $\langle v_i''v_j''(t)\rangle$ and figure 12 for the particle diffusion coefficients $\langle v_i''x_j(t)\rangle$ illustrate this evolutionary dependence in more detail. Figure 10 shows the evolution of $\langle v_1''^2(t)\rangle$, $\langle v_1''v_2''(t)\rangle$ and $\langle v_2''^2(t)\rangle$ compared with their long-term equilibrium values for the case $\beta^{-1} = 1$. The streamwise components

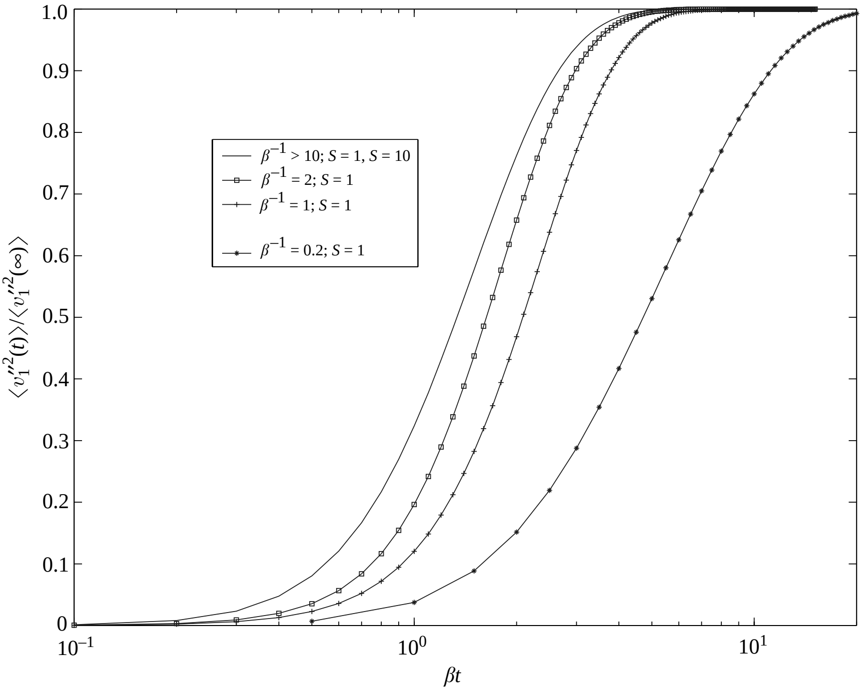

FIGURE 11. Particle mean-square velocity $\langle v_i'' v_j'' \rangle$ as a function of βt for a range of values of β^{-1} and S.

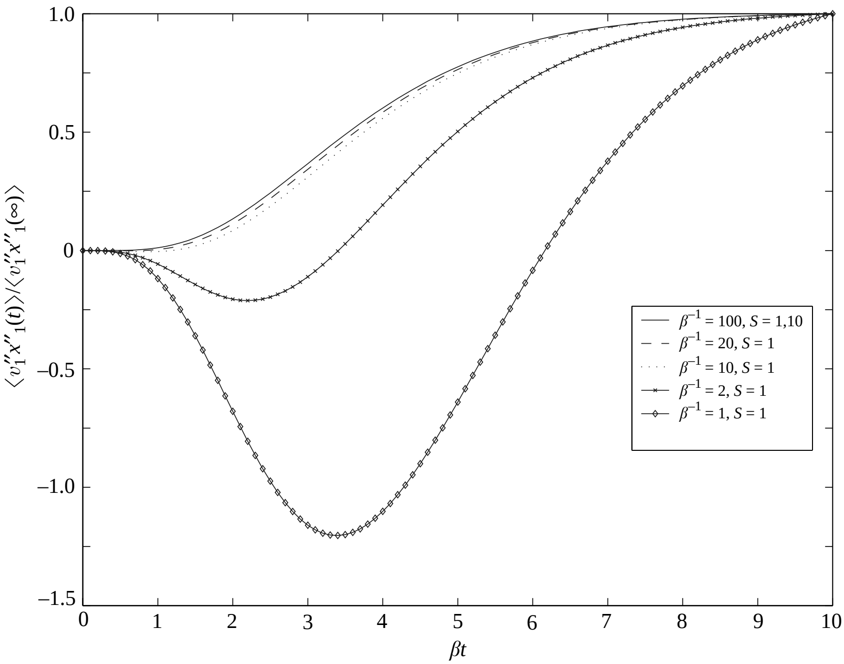

FIGURE 12. Particle diffusion coefficient ratio $\langle v_1'' x_1(t)\rangle / \langle v_1'' x_1(\infty)\rangle$ as a function of βt for range of values of β^{-1} and S.

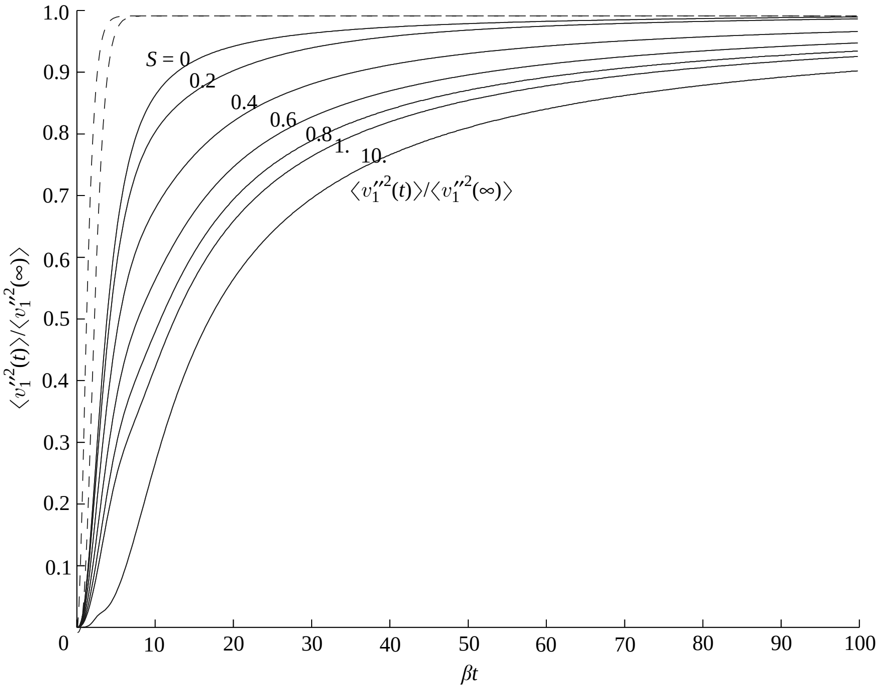

FIGURE 13. Time dependence of $\langle v_1'^2(t)\rangle/\langle v_1''(\infty)\rangle$ compared to $\langle v_1''^2(t)\rangle/\langle v_1''(\infty)\rangle$ as a function of S, $\beta^{-1}=1$.

approach their equilibrium value slower than the cross streamwise components $\langle v_2''^2(t)\rangle$ due to the influence of the strain rate S on the former, the response contracting onto the same curve for large S, i.e. $S>10$ when the deviatoric component makes the dominant contribution. Figure 11 shows that for long response time $\beta \ll 1$ and $\alpha t \gg 1$, the evolution is self-similar in βt and independent of S.

In contrast, based on equation (5.38), we show in figures 13 and 14 the evolution of the covariances of the particle velocity fluctuation $\boldsymbol{v}'$ where we recall that $\boldsymbol{v}'$ is the fluctuation with respect to the mean local particle velocity $\overline{\boldsymbol{v}}$. The evolution of these quantities is the true measure of the way the particle kinetic stresses change with time (see (3.3)). We note from figure 13 that they evolve on a much longer timescale than the corresponding averages associated with $\boldsymbol{v}''$ and though they approach the same values, $\langle v_1'^2\rangle < \langle v_1''^2\rangle$ always, the difference increasing with increasing S but approaching an asymptotic limit.

At first sight this is surprising because we would expect the mean particle velocity to be always less than the corresponding mean carrier flow velocity, which in turn would tend to make $\langle v_1'^2\rangle \geqslant \langle v_1''^2\rangle$. However we note that unlike the statistical independence of $\boldsymbol{v}'$ and $\overline{\boldsymbol{v}}$, this is not the case for v'' and $\overline{\boldsymbol{u}}$ so that in fact

$$\left\langle v_1''^2\right\rangle - \left\langle v_1'^2\right\rangle = \left\langle \overline{v}_1^2\right\rangle - \left\langle \overline{u}_1^2\right\rangle - 2S\left\langle v_1''x_2\right\rangle, \tag{6.19}$$

and that from (6.16) $-2S\langle v_1''x_2\rangle > 0$ and as shown in figure 15 outweighs the negative contribution of $\langle \overline{v}_1^2\rangle - \langle \overline{u}_1^2\rangle$. The same is true of the case when $\beta^{-1}=10$, the curve being the same for $S>10$, though from figure 14 self-similarity in βt for the two sets of curves for $\beta^{-1}=1$ and 10 for $\beta t \gg 1$ does not appear to apply for the range of βt shown in the figure. The self-similarity in βt and independence of S for $S \gg 1$

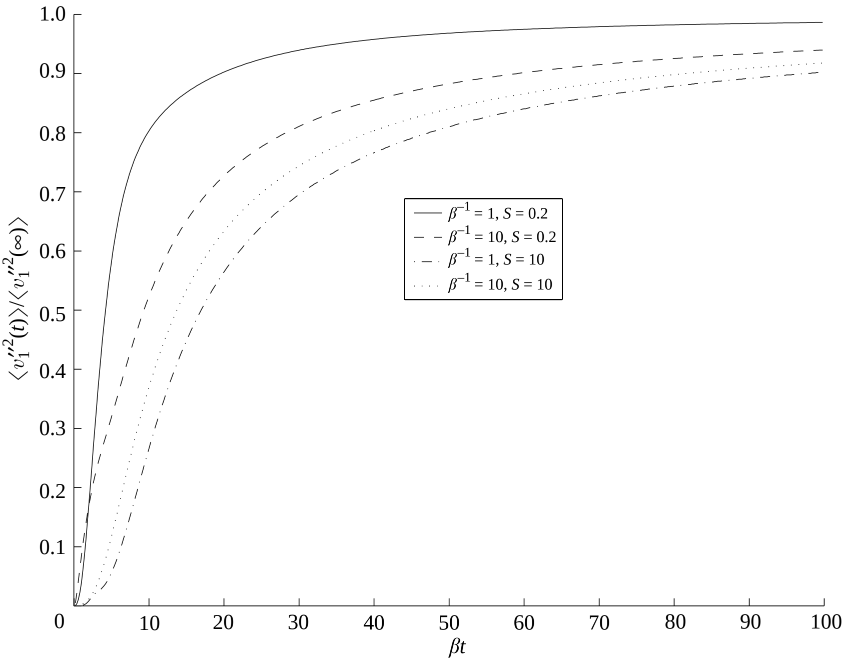

FIGURE 14. $\langle v_1'^2(t)\rangle/\langle v_1''^2(\infty)\rangle$ as a function of βt for values of $\beta^{-1}$and S.

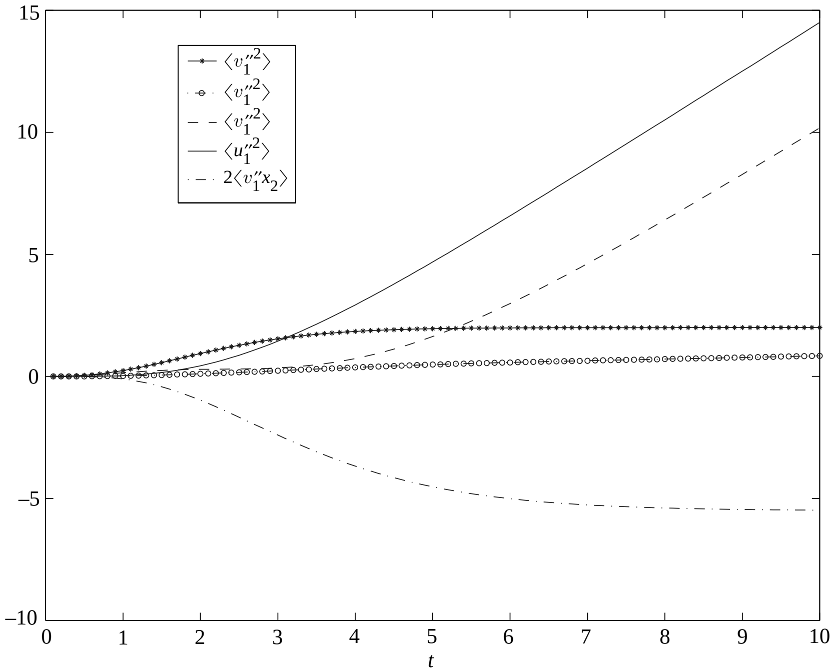

FIGURE 15. Contributions to $\langle v_1'^2(t)\rangle/\langle v_1''^2(\infty)\rangle$ based on equation (6.19) for $S = 1$ and $\beta = 1$.

exhibited by the evolution of $\langle v_1''^2\rangle$ is the same as that of the particle diffusion coefficients $\langle v_1''x_1(t)\rangle$, $\langle v_1''x_2''(t)\rangle$ and $\langle v_2''x_1''(t)\rangle$ shown in figure 12. For these cases, the long-term particle diffusion coefficients in the streamwise direction $\langle v_1''x_1\rangle_\infty < 0$:

however we note from figure 12, that this value is not approached monotonically, the diffusion coefficient being positive to begin with and then changing sign before approaching its equilibrium value. A similar behaviour occurs for $\langle v_2'' x_1''(t)\rangle$.

In the case of both the particle velocity covariances and diffusion coefficients, the contribution of the shear/strain rate is equivalent to an additional driving force which adds to the kinetic energy of the particle and increases the timescale at which this process takes place, whilst, nevertheless, approaching some limiting form. Unlike the influence of β^{-1}, figures 10 and 12 show the influence of S on the timescale to approach equilibrium to be relatively small: S simply determines the relative contribution of the timescales of the deviatoric components to that of the homogeneous contribution which are of the same order. When $\beta^{-1} \gg 1$, the only timescale influencing the process is β^{-1} in real time, hence the self-similarity in βt. In effect the turbulence and the strain rate behave as if they were white noise driving forces on the scale of the particle motion.

It is now appropriate to consider the role of the dispersion coefficients $\langle v_i'' x_j\rangle$ in the total dispersion of the particles as the particle concentration evolves with time. Let us consider first $\langle v_1'' x_1\rangle$ and its contribution to the dispersion in the streamwise direction. Thus we may write

$$\begin{aligned}\langle v_1 x_1\rangle &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle x_1^2\rangle \\ &= S\langle x_1 x_2\rangle + \langle v_1'' x_1\rangle. \qquad (6.20)\end{aligned}$$

For $\langle x_1 x_2\rangle$ we have

$$\begin{aligned}\frac{\mathrm{d}\langle x_1 x_2\rangle}{\mathrm{d}t} &= S\langle x_2^2\rangle + \langle v_1'' x_2\rangle + \langle v_2'' x_1\rangle \\ &\to 2S\langle v_2'' x_2\rangle t \quad \text{for } t\to\infty. \qquad (6.21)\end{aligned}$$

So

$$\langle v_1 x_1\rangle \to S^2\langle v_2'' x_2\rangle t^2 \quad \text{for } t\to\infty. \qquad (6.22)$$

So in the long-term, the contribution of $\langle v_1'' x_1\rangle$, whether it be positive or negative, to the total dispersion in the streamwise direction is negligible. In the short term $t \ll 1$, $\langle v_1 x_1\rangle$ is independent of the strain rate and behaves as $\langle v_1'' x_1\rangle$. However, as we see e.g. in figure 12, for small times $t \ll 1$, $\langle v_1'' x_1\rangle > 0$, in fact $\langle v_1'' x_1\rangle \sim \frac{1}{5}\beta^2 t^4$, whilst $(\mathrm{d}/\mathrm{d}t)\langle x_1 x_2\rangle \sim S\beta^2 t^5$. That is the influence of negative values of the diffusion coefficients $\langle v_1'' x_1\rangle$ is only significant at intermediate time $t \sim 1$, but never exceeds the contribution from the dispersion experienced by the particle arising from the mean shear velocity Sx_2. It would at first appear that the role of the mean shear velocity as a diffusive contribution is in contradiction to its presence as a convective velocity in the equation for the particle flux (6.15). However it is clear that this convective velocity, as encountered by a particle, is itself a random quantity because the particle displacement $x_2(t)$ is random through the influence of the turbulence in the cross-streamwise x_2-direction. Indeed the flux arising from this term, namely $Sx_2\langle\rho\rangle$, can be written more transparently as a diffusive flux,

$$Sx_2\langle\rho\rangle = -S\langle x_2 x_1(t)\rangle\frac{\partial\langle\rho\rangle}{\partial x_1} \qquad (6.23)$$

and the total flux J_1 due to spatial gradients of concentration in the streamwise

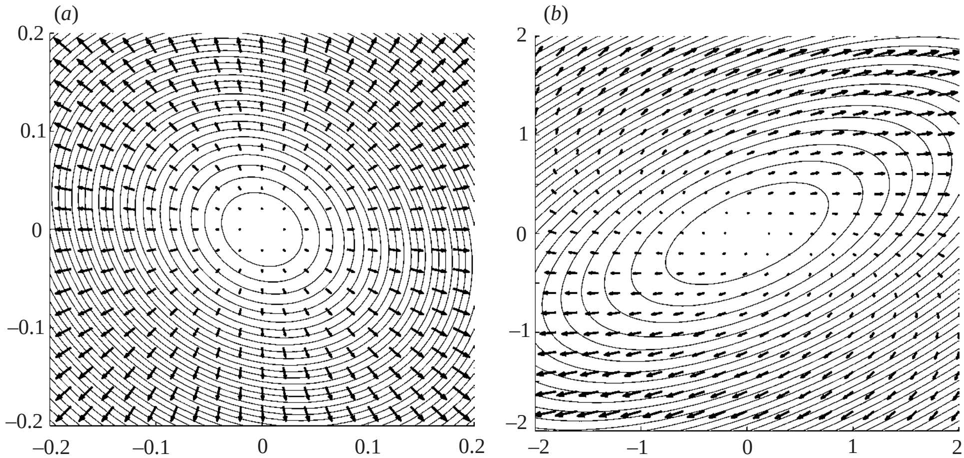

FIGURE 16. Concentration contours and particle mean velocity $\overline{\boldsymbol{v}}$, for $\beta^{-1}=1, S=1$, at (*a*) $\alpha t=2$, (*b*) 6. Concentration contours represent a constant fraction f of the concentration at the centre of the shear, $f=1-0.02n,\ n=1,2,\ldots$.

direction therefore as

$$J_1 = -(S\langle x_2 x_1\rangle + \langle v_1'' x_1\rangle)\frac{\partial\langle\rho\rangle}{\partial x_1}. \tag{6.24}$$

Any concerns that there is a violation of the Second Law of Thermodynamics are unfounded because the total diffusion coefficient is never <0.

6.4. *Evolution of particle mean concentration and particle and carrier mean flow fields*

To see how the asymmetry in the total diffusion coefficients $\langle v_i x_j\rangle$ affects the way the mean particle concentration evolves in space as well as time, we have evaluated the contours of the particle mean concentration at regular intervals of time. The concentration contours in this case are evaluated for a fixed value of f, the fraction of the concentration at the centre of the shear at any given time t. From (5.33), we have at position $\boldsymbol{x}=[r,\theta]$ at time t

$$f=\frac{\langle\rho(r,\theta,t)\rangle}{\langle\rho(0,0,t)\rangle}=\exp\left(-\frac{r^2}{2\det[\langle\boldsymbol{xx}\rangle^{-1}]}\left\{\left\langle x_2^2\right\rangle\cos^2\theta-\langle x_1x_2\rangle\sin 2\theta+\left\langle x_1^2\right\rangle\sin^2\theta\right\}\right) \tag{6.25}$$

where $|\langle\boldsymbol{xx}^{-1}\rangle|$ is explicitly given by

$$\det[\langle\boldsymbol{xx}\rangle^{-1}]=\left\langle x_1^2\right\rangle\left\langle x_2^2\right\rangle-\langle x_1x_2\rangle^2. \tag{6.26}$$

Thus the equation for the concentration contours shown e.g. in figure 16 is

$$r^2=-2\log(f)\det[\langle\boldsymbol{xx}\rangle^{-1}]/\left\{\left\langle x_2^2\right\rangle\cos^2\theta-\langle x_1x_2\rangle\sin 2\theta+\left\langle x_1^2\right\rangle\sin^2\theta\right\} \tag{6.27}$$

where f refers to a fixed value of the ratio $\langle\rho(r,\theta t)\rangle/\langle\rho(0,0,t)\rangle$. Figure 16 shows the concentration contours at times $\alpha t=2$ and 4 where the concentration contours are for $f=1-n\Delta f,\ n=1,2\ldots$, with $\Delta f=0.02$. The contours are ellipses which possess the same principal axis which rotate and expand with time. The angle the major principle axis of the ellipses makes with the x_1- axis in the streamwise direction is

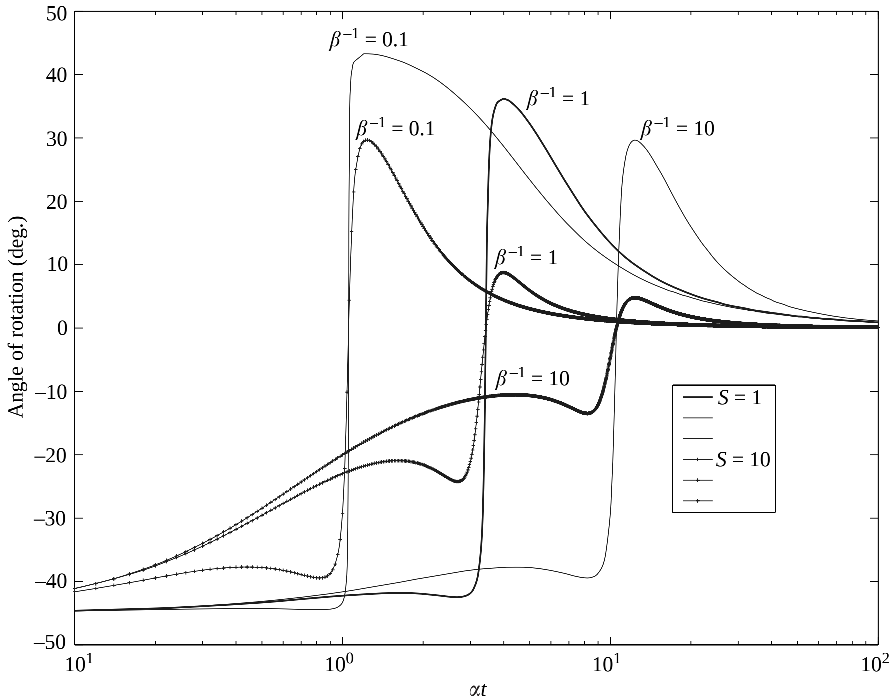

FIGURE 17. Angle of rotation of major principle axis of concentration contours with respect to the streamwise direction.

given by

$$\theta = \frac{1}{2}\tan^{-1}\left(\frac{2\langle x_1 x_2\rangle}{\langle x_1^2\rangle - \langle x_2^2\rangle}\right) \tag{6.28}$$

and this value is shown in figure 17 as a function of time for various values of β^{-1} and S. It is clear that for each case considered, the major principal axis initially is at $\theta = -45^\circ$ and remains roughly at this value for an initial period depending on the value of β^{-1}, θ then switching very rapidly to a positive peak value after which it decays away to zero asymptotically as $t \to \infty$. The time at which θ switches from negative to positive value increases with β^{-1}, the transition becoming more gradual. The transition is independent of S, the value of S reducing the value of the peak value θ before it decays away to zero.

The way in which the mean particle velocity field shown e.g. in figure 16 evolves with time can be analysed more comprehensively by decomposing it into its symmetric strain and vorticity components and considering the way in which these evolve with time for different values of the particle response time β^{-1} and strain rate S. Thus if according to (5.35) the components of $\overline{\boldsymbol{v}}$ are given by

$$\overline{v}_i = S_{p,ij} x_j$$

where

$$\boldsymbol{S}_p = \langle \boldsymbol{v}^* \boldsymbol{x}^* \rangle \langle \boldsymbol{x}^* \boldsymbol{x}^* \rangle^{-1}$$

then we can represent $\overline{\boldsymbol{v}}$ by

$$\overline{\boldsymbol{v}} = \boldsymbol{S}_p^+ \cdot \boldsymbol{x} + \boldsymbol{\omega} \times \boldsymbol{x}$$

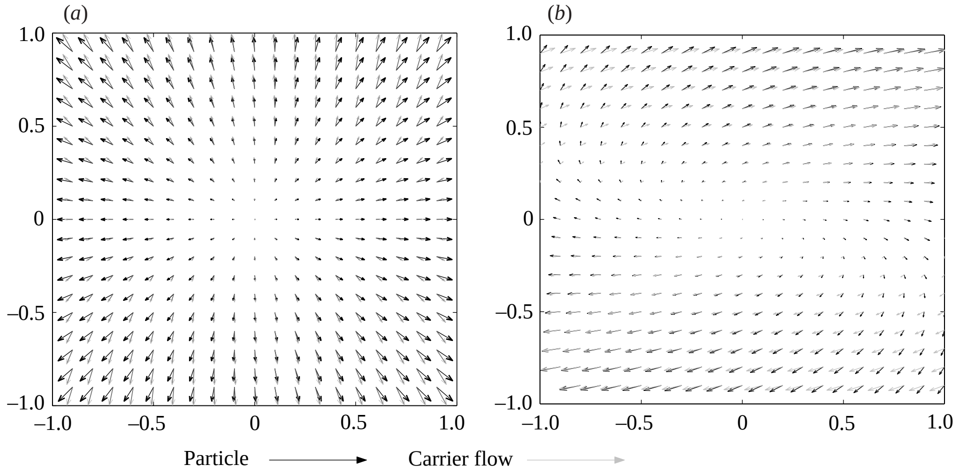

FIGURE 18. Mean particle and mean flow velocity (encountered by particle) fields for developing shear for $\beta^{-1}=1$, $S=1$, at (*a*) $\alpha t=1$ and (*b*) 6.

where $\boldsymbol{S}^{+}$ is a symmetric strain rate tensor whose components are

$$S^{+}_{p,ij} = \tfrac{1}{2}(S_{p,ij} + S_{p,ji})$$

and $\boldsymbol{\omega}=\frac{1}{2}\nabla\times\overline{\boldsymbol{v}}$ which in this instance is a vector in the x_3-direction with magnitude ω given by

$$\omega = \tfrac{1}{2}(S_{p,21} - S_{p,12}).$$

In the long-term $S^{+}_{p,12}=-\omega=\frac{1}{2}S$. In turn $\boldsymbol{S}^{+}_{p}$ has then been characterized by its eigenvalues s_1 and s_2, being the normal rates of expansion/compression along the principal axes of $\boldsymbol{S}^{+}_{p}$ defined by the corresponding eigenvectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ of $\boldsymbol{S}^{+}_{p}$ respectively which are perpendicular to one another.

Using equation (5.64), we have also evaluated $\overline{\boldsymbol{u}}$, the mean carrier flow velocity encountered by a particle at the same time. Figure 18 shows the forms of both $\overline{\boldsymbol{v}}$ and $\overline{\boldsymbol{u}}$ at $\alpha t=1$ and 6 which can be compared with the particle mean concentration contours at the same times shown in figure 16. It is evident that $\overline{\boldsymbol{v}}$ lags behind $\overline{\boldsymbol{u}}$, the difference reducing with increasing time but increasing with distance from the centre of the shear. The flow field in both cases is radial-like to begin with and highly expansive (e.g. for $\alpha t=1$) and then becomes more shear-like as both flow fields align with the underlying simple shear flow (e.g. for $\alpha t=6$).

Figure 19 shows the evolution of both the particle and carrier mean flow fields (encountered by the particle) in terms of their vorticity ω and strain rate $S^{+}_{p,12}$. In particular ω and $S_{p,12}$ for the carrier flow approach their equilibrium values much more rapidly than those for the particles. Both particle and carrier mean flow fields have rotational components which are anti-clockwise to begin with, i.e. $\omega>0$, but change sign to accommodate the change from a radial outward flow (but in a preferred direction) to eventually a simple shear flow. In the case of the carrier flow (encountered by the particle) the initial rotation is much greater than for the particle mean flow.

Comparing this with the angle of rotation of the principal axis of the concentration contours in figure 17, we note that the initial rotation of the concentration contours

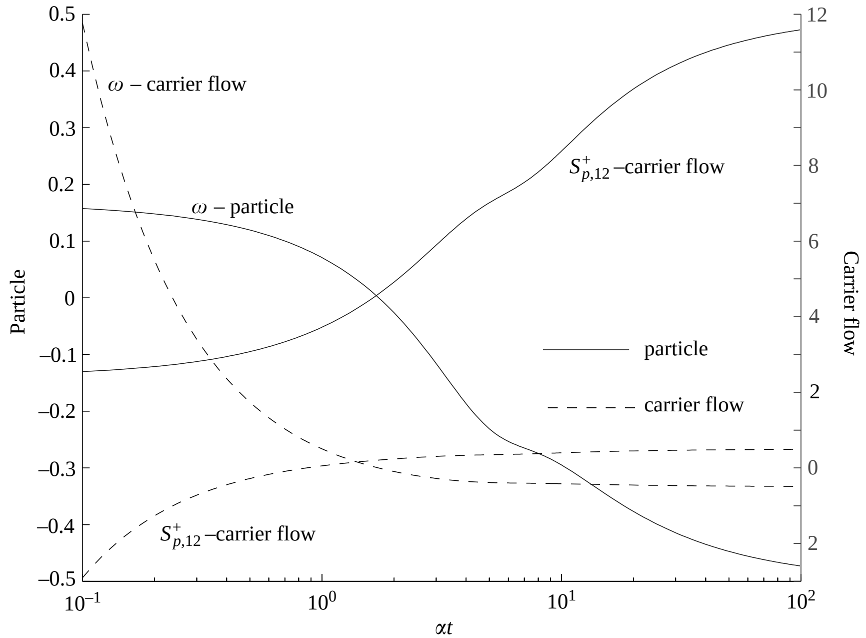

FIGURE 19. Symmetric strain rates S^+_{12} and rotation ω of particle and carrier flow (encountered by particle) mean velocity flow fields for $\beta^{-1} = 1$, $S = 1$.

is in the same direction as the rotational component of the mean particle velocity. As we might expect with particles of greater relaxation time, the threshold time for transition from an outward radial flow $s_2/s_1 > 0$ to a straining flow $s_2/s_1 < 0$ is greater and the timescale to approach the long-term value of $s_2/s_1 = 0$ is greater also. For the case of $\beta^{-1} = 1$, $S = 1$ when $\alpha t \backsim 1.7$, $S^+_{p,12}$ is zero, i.e. at this time the principal axes of the symmetric straining flow of the particle are in the $-x_1, x_2$-directions. This is close to the time when $\omega = 0$, so that in this case, the mean particle flow field is close to a symmetric straining flow: however we can see from figure 20 that at this time, the ratio of the strain rates s_2/s_1 is very close to unity, indicating that the strain flow components, as with the mean particle flow itself, are still very close to a radial outward (expansive) flow. Note from figure 21 that the strain ratio s_2/s_1 is at a peak value when this occurs, from which it decays asymptotically to its long-term value of -1.

However, we note that for the case $\beta^{-1} = 1$ during the initial phase $1 > s_2/s_1 > 0$, the angle of rotation ψ of the principal strain rate axis $\boldsymbol{e}_1$ overshoots its long-term equilibrium value of $-135°$, a property also shared by the case when $\beta^{-1} = 10$, reaching a minimum at a somewhat lower value than that for $\beta^{-1} = 1$. Figure 21 contrasts the behaviour of the strain rates with time for $S = 1$ with that for $S = 10$. It is noticeable that the peak value at which $S^+_{p,12} = 0$ is much more sharply defined for $S = 10$, but at a lower but still positive value than in the case for $S^+_p = 0$. It is important to note also that throughout the process the strain rate s_1 in the $\boldsymbol{e}_1$-direction is always positive (expansive) and whilst the strain rate s_2 in the $\boldsymbol{e}_2$-direction perpendicular to $\boldsymbol{e}_1$ is negative, the divergence of $\overline{\boldsymbol{v}}$, $\nabla \cdot \underline{\boldsymbol{v}} = s_1 + s_2$ is always >0. That is the particle mean concentration decreases everywhere as time progresses, so there is no violation of the Second Law of Thermodynamics.

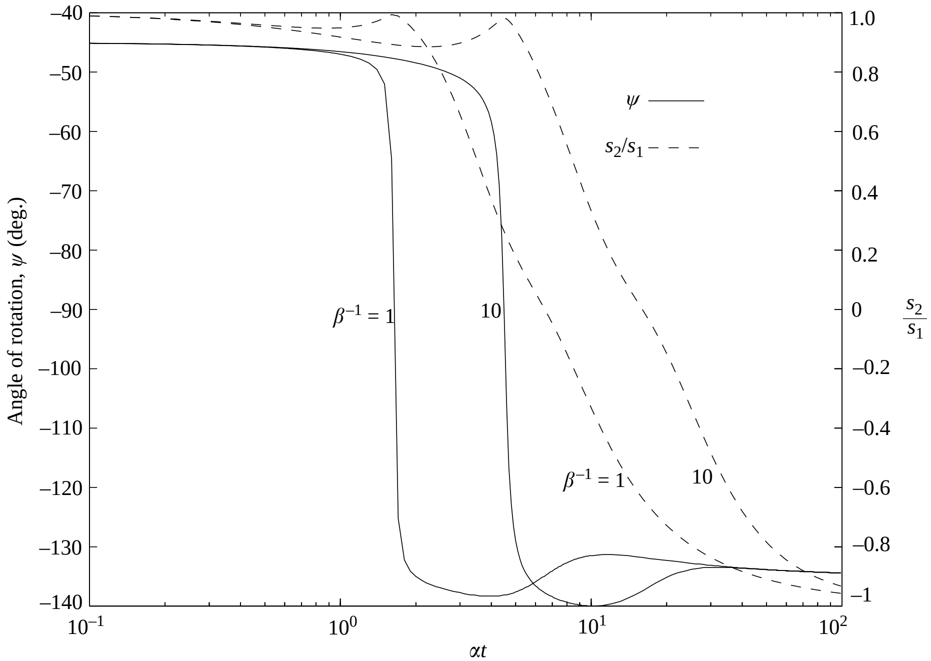

FIGURE 20. Angle of rotation ψ of $\boldsymbol{e}_1$-principal axis of symmetric shear component $\boldsymbol{S}_p^+$ of mean particle velocity field $\overline{\boldsymbol{v}}$ and ratio of corresponding eigenvalues (strain rates) s_2/s_1 for $S=1$.

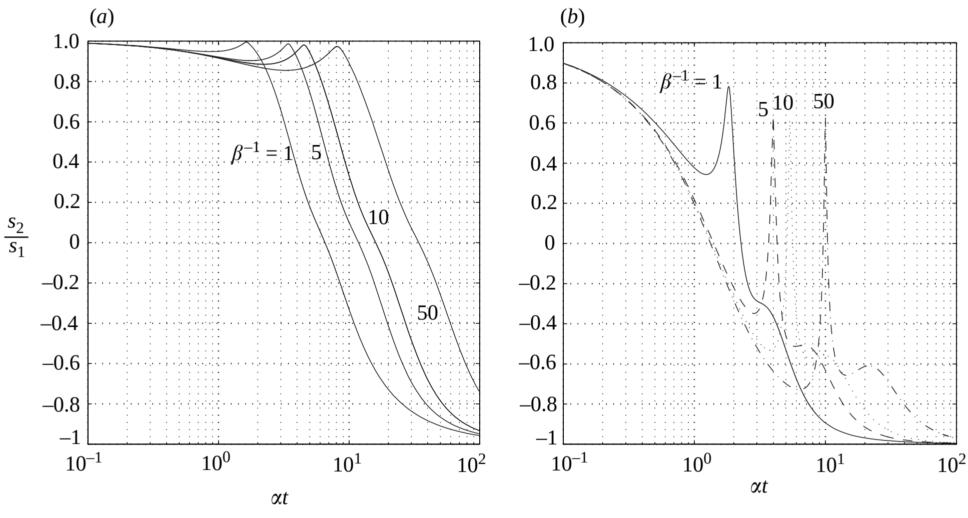

FIGURE 21. Ratio of strain rates s_2/s_1 of symmetric shear component S^+ of mean particle velocity field $\overline{\boldsymbol{v}}$ for (a) $S=1$, (b) 10.

7. Comments on passive scalar dispersion in a simple shear flow

We recall that the discrepancy between the two PDF formulations for the particle diffusion coefficients in a simple shear has its origin in certain assumptions that were made for passive scalar diffusion in the same flow. In this section we will consider these assumptions in more detail since they have some bearing on the general use of algebraic Reynolds stress models for passive scalar diffusion in turbulent shear flow. Rogers *et al.* (1989) carried out numerical simulations of passive scalar diffusion of temperature in a homogeneous turbulent shear flow. In particular they analysed the form of the scalar heat flux in relation to the mean scalar gradient of the temperature and found that a gradient transport model was appropriate in combination with a set of turbulent diffusion coefficients in the same way as that represented by equation (6.15) except that the form of the diffusion coefficients remained unspecified to begin with. They then used their simulations to fit a dimensionless model for the diffusion coefficients which was based on certain assumptions. It is instructive to recall precisely what those assumptions were, on what basis they were made and in what way they are similar to the neglect of the inertial acceleration term in the momentum equation (4.5). In so doing, it is clear that we are addressing a more fundamental question relevant to both single and multiphase flows alike namely, *to what extent in the long-term can a momentum equation be interpreted as a convection–diffusion equation*?

The averaged equations governing the flow velocity $\boldsymbol{u}(\boldsymbol{x},t)$ and transport of a passive scalar $T(\boldsymbol{x},t)$ (e.g. temperature) in an incompressible flow with material density ρ_f and kinematic viscosity ν_f are

$$\frac{\partial\langle u_i\rangle}{\partial x_i}=0, \tag{7.1}$$

$$\frac{\mathrm{D}\langle u_i\rangle}{\mathrm{D}t}=-\frac{\partial\langle u_j''u_i''\rangle}{\partial x_j}-\rho_f^{-1}\frac{\partial\langle p\rangle}{\partial x_i}+\nu_f\frac{\partial^2\langle u_i\rangle}{\partial x_j\partial x_j}, \tag{7.2}$$

$$\frac{\mathrm{D}\langle T\rangle}{\mathrm{D}t}=\frac{\partial}{\partial x_i}\gamma\frac{\partial\langle T\rangle}{\partial x_i}-\frac{\partial}{\partial x_i}\langle T''u_i''\rangle+\Sigma, \tag{7.3}$$

where $p(\boldsymbol{x},t)$ denotes the instantaneous pressure, $T''(\boldsymbol{x},t)$ the fluctuating component of $T(\boldsymbol{x},t)$ with respect to a mean $\langle T\rangle$, Σ a source term assumed to be steady and uniform or linear in $\boldsymbol{x}$ in the cases considered; γ is the molecular diffusivity of the passive scalar supposed constant in time and spatially uniform. For homogeneous turbulence in a uniform mean shear given by (5.4), the equation for the mean scalar flux $\langle T''u_i''\rangle$ is

$$\frac{\mathrm{D}\langle u_i''T''\rangle}{\mathrm{D}t}=-\langle u_i''u_j''\rangle\frac{\partial\langle T\rangle}{\partial x_j}-\langle T''u_j''\rangle\frac{\partial\langle u_i\rangle}{\partial x_j}+\psi_i \tag{7.4}$$

where ψ_i is a source term involving the pressure scalar gradient covariance and a dissipation term due to molecular viscosity and diffusion involving the covariance of both flow velocity and scalar gradients, namely

$$\psi_i=\rho^{-1}\left\langle p\frac{\partial T''}{\partial x_i}\right\rangle-(\nu+\gamma)\left\langle\frac{\partial u_i''}{\partial x_j}\frac{\partial T''}{\partial x_j}\right\rangle \tag{7.5}$$

cf. the dissipation terms in the transport equation for the turbulent kinetic energy. The ways in which ψ_i and $\mathrm{D}\langle T''u_i''\rangle/\mathrm{D}t$ are modelled are crucial to the way in which the scalar flux can be regarded as a gradient diffusion term as part of a realizable statistical process and to the value and relationships of the corresponding diffusion coefficients. On the basis of a number of experiments and heuristic arguments, it is assumed that ψ_i is a negative quantity proportional to the scalar flux with a constant of proportionality $\sim-(\epsilon/q^2)$ where ϵ is the turbulent dissipation rate and q^2 the turbulent kinetic energy per unit mass. In so doing therefore, one can write the scalar flux equation (7.4) in the form

$$\frac{\mathrm{D}\langle u_i''T''\rangle}{\mathrm{D}t} = -\langle u_i''u_j''\rangle\frac{\partial\langle T\rangle}{\partial x_j} - \langle T''u_2''\rangle S\delta_{i1} - \frac{1}{\tau}\langle T''u_i''\rangle \tag{7.6}$$

where τ is some timescale typical of the large-scale turbulent motion. Compare this with Pope's GLM equation for the passive scalar flux for a simple shear, namely

$$\langle\rho\rangle\frac{\mathrm{D}}{\mathrm{D}t}\overline{u_i''} = -\langle u_i''u_j''\rangle\frac{\partial\langle\rho\rangle}{\partial x_j} - \langle\rho u_2''\rangle S\delta_{i1} - \alpha_{ij}\langle\rho u_j''\rangle. \tag{7.7}$$

In fact in the long-term limit for a Gaussian process, which is true for the GLM equation in a uniform shear, the local time derivative of the mean carrier flow velocity dominates the convective term in the substantial derivative term on the left-hand side of (7.7), so apart from the assumption of local isotropy surrounding the relationship between scalar flux and ψ_i, equation (7.6) is compatible with Pope's GLM equation in the long-term limit. However, on the basis of the results of their simulations, Rogers *et al.* make the further assumption that in the long-term limit

$$\frac{\mathrm{D}\langle u_i''T''\rangle}{\mathrm{D}t} \approx \text{scalar} \times \langle u_i''T''\rangle, \tag{7.8}$$

that scalar being typically $\sim\tau^{-1}$, so the scalar flux equation reduces to

$$0 = -\langle u_i''u_j''\rangle\frac{\partial\langle T\rangle}{\partial x_j} - \langle T''u_2''\rangle S\delta_{i1} - C_D\frac{1}{\tau}\langle u_i''T''\rangle \tag{7.9}$$

where C_D is some dimensionless constant. Now whilst (7.9) is not based on neglect of the acceleration term, it is however incompatible with a Gaussian process in which the passive scalar is convected by an underlying velocity field with mean shear component and a random component which is stationary and homogeneous. More succinctly, it is incompatible with a Gaussian process for $[\boldsymbol{u}(t), \boldsymbol{x}(t)]$ where $\boldsymbol{u}(t)$ and $\boldsymbol{x}(t)$ are the velocity and position of a fluid element as it moves through the velocity flow field. In this case the scalar fluxes are related to the mean scalar gradient via diffusion coefficients that are global averages of the dispersion process, in particular to $\langle u_i''(t)x_j(t)\rangle$ or to specific averages $\langle u_i(\boldsymbol{x}, t)\Delta\boldsymbol{x}(\boldsymbol{x}, t \mid 0)\rangle$ about a point $\boldsymbol{x}, t$ going backwards in time. Given then that, for self-consistency, the transport equation for $\langle u_i''T''\rangle$ must generate the same mean scalar gradient form for $\langle u_i''T''\rangle$ with the same global averages for the associated diffusion coefficients, this implies that the acceleration term must itself be related to the mean scalar gradient rather than to the scalar itself, the latter assumption leading to a non-realizable statistical process. All of this reasoning of course neglects the role of molecular diffusion which though small, in general complicates the issue: however it could well help to make the latter assumption in (7.8) more acceptable in terms of realizability. It is worth noting that a similar assumption to that given in (7.8) has been used in passive scalar diffusion in inhomogeneous shear flows (Gibson & Launder 1976) where this assumption may be even more questionable.

The analysis of Tavoularis & Corrsin (1985) which the authors refer to as 'passive scalar diffusion using mostly material coordinates', is an evaluation of $\langle u_i''(t)x_j(t)\rangle$ in terms of time integrals involving Lagrangian autocorrelations $\langle u_i''(0)u_j''(t)\rangle$ along flow fluid point trajectories, specific forms being explicitly evaluated using an exponential decay for this autocorrelation when comparing their predictions with their experimental measurements. Their analysis is entirely compatible with the results we have presented here for the GLM approach used for both particle and fluid point dispersion except that in the GLM approach the statistics we use, e.g. the Lagrangian autocorrelation $\langle u_i''(0)u_j''(t)\rangle$, are part of the model for the shear flow and not freely prescribed inputs to the calculation. The significant feature of their analysis was the recognition that the streamwise diffusion coefficient could be negative, a result consistent with the simple form of GLM used here.

8. Summary and conclusions

The purpose of this paper is two-fold: first to resolve the apparent conflict between the two PDF approaches and secondly to provide exact solutions to the dispersion of particles in a simple unbounded shear flow based on the GLM set of equations due to SDM. This analysis not only served to highlight the source and magnitude of the discrepancy graphically but showed precisely how the dispersion scaled with time and in what way it depended upon the particle inertia (Stokes number) and the strain rate. The source of the discrepancy was identified as the neglect of the inertial acceleration term in the transport equation for the mean carrier flow velocity encountered by the particle, i.e. the first term on the left-hand side of (4.5), which is incompatible with a Gaussian process: for a Gaussian process this term is linear in the mean particle concentration gradient and is of the same order as the other concentration gradient terms in the equation. When the correct form for the inertial acceleration term is introduced into the equation, the fluid-particle dispersion coefficient has the correct form for a Gaussian process and is identical to the form used in the KM approach.

Whilst these two approaches are compatible, an important difference between them is that the GLM approach provides a model for particle transport and at the same time a model for the turbulence encountered by the particle which encompasses, in the limit of very small particles, the turbulence of the carrier flow itself. In the KM approach, this information must be prescribed independently either on the basis of experiment or from a separate model like the GLM. Given however the same information in the appropriate form, both approaches should give the same results for a process which is Gaussian.

In analysing the dispersion of particles in the GLM for particle dispersion in a simple shear flow, we chose the simplest GLM in which the response time of the carrier flow was isotropic and homogeneous. We began by evaluating the long-term values of the fluid-particle diffusion coefficients using the particle response method used in the KM approach to show that both methods were the same. This requires information on the autocorrelation of the carrier flow velocity fluctuations along a particle trajectory, i.e. $\langle u_i''(t)u_j''(t+s)\rangle_{t\to\infty}$ which was determined from the SDM equations. In this model set of equations, these autocorrelations depend on the strain rate S normalized on the timescale of the turbulence and are independent of particle inertia. In particular the off-diagonal components possess the interesting property that, although stationary in time, they are not symmetric in the time difference s (see (6.5) and figure 2). Significantly the streamwise components of both the velocity and spatial diffusion coefficients are both negative for a significant range of the particle response time depending on the strain rate: this includes the case of very small particles (zero response times).

In the case of the particle velocity covariance and particle diffusion coefficients, their long-term values as well as their time dependence (including the approach to equilibrium) were found by solving numerially the coupled set of momentum equations of the PDF equation for $\langle P(\boldsymbol{v}, \boldsymbol{u}, \boldsymbol{x}, t)\rangle$. Relatively simple algebraic expressions were obtained for the long-term values for both in terms of S and β^{-1}. Regarding the influence of the normalized strain rate S on the particle velocity covariance, as in previous calculations, the streamwise fluctuating velocity covariance is increased by the shear and also by increasing the particle response time; the deviatoric components of the off-diagonal covariances are proportional to the strain rate with a turbulent Schmidt number which is zero for particles which follow the flow and tends to 1/2 for particles with increasingly large response times (equation(6.13)).

Like fluid-particle diffusion coefficients, depending on the value of β^{-1} and S, the spatial particle diffusion coefficients were also negative. However in this model negative values were always the case when $S > 0.892$ irrespective of β^{-1} and always negative for fluid point (passive scalar) motion if $S > \sqrt{2/3}$. In contrast the corresponding values with neglect of the inertial acceleration term are mostly but not always positive as is the case for the fluid-particle diffusion coefficients. We recall that the origin of these negative diffusion coefficients is linked to the influence of the shear itself and the creation of positive Reynolds stresses both for the carrier flow and the dispersed phase. More particularly there are two contributions to the particle diffusion coefficient $\langle v_1'' x_1 \rangle$: a positive contribution from displacements arising from turbulent fluctuations of the carrier flow in the streamwise direction, and the other directly from the shear itself because particles crossing the mean shear flow with positive velocities in the cross-stream direction will be carrying negative streamwise velocity fluctuations and associated with negative streamwise displacement and vice versa for particles moving in the negative cross-streamwise direction. The two contributions oppose one another and whilst both contributions depend on the shear, in this particular GLM, the negative contribution outweighs the positive as the shear is increased.

We further discussed the role of negative diffusion coefficients in the context of a particle flux made up of a convective flux and a diffusive flux given by equation (6.15), noting that the convective flux in the streamwise direction behaved like a diffusive flux since the net convection in the streamwise direction depended on how far the particle had diffused in the cross-stream direction. So the whole dispersion process for particles released from the centre of the shear could be represented by a gradient diffusion process with total diffusion coefficients $\langle v_i x_j \rangle$ that depend upon the convection imposed by the mean shear itself and the contribution of the actual turbulence both in the streamwise and cross-streamwise directions, equation (6.20): whilst these later contributions may reduce the value of total streamwise diffusion coefficient, it is always positive.

The role of these diffusion coefficients in controlling the dispersion process was made more transparent when we considered the evolution of the particle concentration field and its relation to the underlying mean velocity fields of the particles themselves and that of the carrier flow velocities encountered the particles, the latter features being unique to this analysis. The contours of mean particle concentration were seen as ellipses sharing a common set of principal axes at any give time. These principal axes rotated as the concentration dispersed, first anti-clockwise very rapidly and then clockwise as the major principal axis eventually aligned with the streamwise direction of the shear (see figure 17). To characterize the behaviour of the underlying mean velocity fields more succinctly, they were decomposed into their symmetric strain rate and vorticity components. The symmetric strain rate component was then resolved in terms of the normal strain rates (its eigenvalues) along its principal axes (eigenvectors). We then considered how these quantities changed with time as a function of normalized strain rate and particle inertia. Both particle and carrier mean flow fields have rotational components which are anti-clockwise to begin with and then change sign, following the same behaviour as the rotation of the principal axes of the concentration contours. In the initial phase of the dispersion, both mean flow fields are radially outward, changing to a straining flow with one of the principal strain rates becoming compressional. However the total divergence of the mean particle velocity field is always >0, i.e. the concentration decreases everywhere and for all time.

In the final section we considered in detail the assumptions that lead to the discrepancy between the two formulations of the passive scalar dispersion in uniform shear flow since they have some bearing on the general use of algebraic Reynolds stress models for passive scalar diffusion in turbulent shear flow. It was shown that the discrepancy arose not through neglect of the local acceleration term in the transport equation of the diffusive flux but in assuming it to be proportional to the flux itself rather than to the mean scalar gradient as it would be for a Gaussian process. In more general terms, for this flow the diffusion coefficient and the ensemble average $\langle u_i''(t)x_j(t)\rangle$ must be identical to one another, which is incompatible with the assumption of proportionality of the local net acceleration term and the scalar flux and hence to a realizable process.

What then are the deficiencies in the GLM approach applied to this simple flow and to dispersed flows in general? It is clear that neglect of the contribution of the fluctuating strain rate, namely $(\boldsymbol{v}-\boldsymbol{u})\cdot\partial\boldsymbol{u}''/\partial\boldsymbol{x}$ in the SDM (2.14) or assuming that this term is absorbed into the white noise function, is an assumption that needs closer examination. We have seen that as a result, the autocorrelations of the carrier flow velocity fluctuations $\langle u_i''(t)u_j''(t+s)\rangle_{t\to\infty}$ are independent of the particle inertia β. Furthermore they are independent of any drift we might impose on the particles as they disperse in the shear, i.e. there is no crossing trajectory effect. This can be traced to the use of a white noise function in time, i.e. the fluctuating carrier flow velocity generated by a GLM has no spatial structure: Eulerian timescales are the same as Lagrangian timescales. Inclusion of the fluctuating shear in the SDM equation and finding suitable closure approximation for terms like $\langle \rho u_j''\partial u_i''/\partial x_j\rangle$ that subsequently appear in the momentum equation for the carrier phase equation (4.3) may well introduce such additional features and is a subject for further investigation.

A significant part of the work described in this paper was carried out in the Institute for Environment and Sustainability at the European Joint Research Centre, Ispra, Italy when the author was supported by a Marie Curie Experienced Researcher Fellowship of the European Community programme, Contract No. 20618-2003-03 P1B40 ISP IT

Appendix. Response functions for a simple shear flow

To simplify the analysis and reduce the number of variables we assume that all times scale on α^{-1} and velocities on $\langle u_2''^2\rangle^{1/2}$, the r.m.s. velocity of the carrier shear flow in the cross-streamwise direction which is unaffected by the shear. So in that case, the SDM equations of motion for u_i'' become

$$\left.\begin{aligned}\frac{\mathrm{d}u_1''}{\mathrm{d}t} &= -u_1'' - u_2''S + f_1(t),\\ \frac{\mathrm{d}u_2''}{\mathrm{d}t} &= -u_2'' + f_2(t),\end{aligned}\right\} \tag{A 1}$$

so in the case of homogeneous shear flow, the SDM equation for $\boldsymbol{u}''$ shows $\boldsymbol{u}''$ to be independent of particle inertia β, i.e. the statistics are the same as for a fluid point of the carrier flow. For this set of equations we define response functions $G^{u''}_{ji}$ where $j = 1, 2$ corresponds to an impulsive force $\delta_{ij}\delta(t)$ applied to the right-hand side of the equation for u''_j (in place of $f_j(t)$) and $i = 1$ and 2 corresponds to the resulting values of u''_i respectively. So for the application of a driving force $f_j(t)$, we have

$$u''_i(t) = \int_0^t f_j(s) G^{u''}_{ji}(t-s)\,\mathrm{d}s.$$

Solution of the set of equations (A 1) with $f_i(t) = \delta_{ij}\delta(t)$ gives

$$\boldsymbol{G}^{u''} = \begin{pmatrix} \mathrm{e}^{-t} & 0 \\ -St\,\mathrm{e}^{-t} & \mathrm{e}^{-t} \end{pmatrix}. \tag{A 2}$$

This set of response functions is to be taken with the set of response functions G^x_{ij} for the particle displacement in the shear as defined earlier in equations (5.30) and are the solutions of the equations

$$\left.\begin{aligned} \frac{\mathrm{d}x_1}{\mathrm{d}t} &= v_1, \\ \frac{\mathrm{d}x_2}{\mathrm{d}t} &= v_2, \\ \frac{\mathrm{d}v_1}{\mathrm{d}t} &= -\beta v_1 + \beta S x_2 + \delta_{j1}\delta(t), \\ \frac{\mathrm{d}v_2}{\mathrm{d}t} &= -\beta v_2 + \delta_{j2}\delta(t), \end{aligned}\right\} \tag{A 3}$$

where

$$G^x_{j1}(t) = x_1(t),\ \ G^x_{j2}(t) = x_2(t), \dot{G}^x_{j1}(t) = v_1(t), \dot{G}^x_{j2} = v_2(t).$$

The solutions are given in equations (5.33)–(5.35).

REFERENCES

Buyevich, Y. 1971 Statistical hydromechanics of disperse systems. Part 1. Physical background and general equations. *J. Fluid Mech.* **49**, 489–507.

Buyevich, Y. 1972*a* Statistical hydromechanics of disperse systems. Part 2. Solution of the kinetic equation for suspended particles. *J. Fluid Mech.* **52**, 345–355.

Buyevich, Y. 1972*b* Statistical hydromechanics of disperse systems. Part 3. Pseudo-turbulent structure of homogeneous suspensions. *J. Fluid Mech.* **56**, 313–336.

Derevich, I. V. & Zaichik, L. I. 1988 Precipitation of particles from a turbulent flow. *Izv. Akad. Nauk SSR, Mekh. Zhid. i Gaza*, 96–104.

Gibson, M. M. & Launder, B. E. 1976 On the calculation of horizontal turbulent, free shear flows under gravitational influence. *Trans. ASME J. Heat Transfer* **98**, 81–87.

Haworth, D. C. & Pope, S. B. 1986 A generalized Langevin model for turbulent flow. *Phys. Fluids* **29**, 387–405.

Hyland, K. E., Reeks, M. W. & McKee, S. 1999*a* Derivations of a p.d.f. kinetic equation for the transport of particles in turbulent flow. *J. Phys: Math Gen.* **32**, 6169–6190.

Hyland, K. E., Reeks, M. W. & McKee, S. 1999*b* Exact analytic solutions to turbulent particle flow equations. *Phys. Fluids* **11**, 1249–1261.

Pope, S. B. 1994 Lagrangian PDF methods for turbulent flows. *Annu. Rev. Fluid Mech.* **26**, 23–63.

Pozorski, J. & Minier, J.-P. 1998 Probability density function modelling of dispersed two-phase turbulent flows. *Phys. Rev.* E **59**, 855–863.

Reeks, M. W. 1980 Eulerian Direct Interaction applied to the statistical motion of particle in a turbulent fluid. *J. Fluid Mech.* **83**, 529–546.

Reeks, M. W. 1991 On a kinetic equations for the transport of particles in turbulent flows. *Phys. Fluids* A **3**, 446–456.

Reeks, M. W. 1993 On the continuum equations for dispersed particles in nonuniform flows. *Phys. Fluids* A **5**, 750–761.

Simonin, O., Deutsch, E. & Minier, J.-P. 1993 Eulerian prediction of the fluid/particle correlated motion in turbulent two-phase flows *Appl. Sci. Res.* **51**, 275–283.

Swailes, D. C. & Derbyshire, K. F. F. 1997 A generalised Fokker-Planck equation for particle transport in random media. *Physica* A **242**, 38–48.

Swailes, D. C., Derbyshire. K. F. F. & Reeks, M. W. 1995 Analysis of particle dispersion using a p.d.f. equation; results for simple shear and rotating flows. *Gas-Particle Flows: ASME Summer Meeting, Hilton Head Island, SC, August*. ASME FED-Vol. 228, pp. 257–263.

Rogers, M. M., Mansour, N. N. & Reynolds, W. C. 1989 An algebraic model for the turbulent flux of a passive scalar. *J. Fluid Mech.* **203**, 77–101.

Tavoularis, S. & Corrsin, S. 1985 Effects of shear on the turbulent diffusivity tensor. *Intl J. Heat Mass Transfer* **28**, 265–276.

Zaichik, L. I. 1991 Modelling of particle dynamics and heat transfer using equations for first and second moments of velocity and temperature fluctuations. In *Eighth Intl Symp. on Turbulent Shear Flows, Technical University of Munich*, pp. 10-2-1–10-2-6.