

Criteria for the selection of stochastic models of particle trajectories in turbulent flows

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Many different random-walk models of dispersion in inhomogeneous or unsteady turbulence have been proposed and several criteria have emerged to distinguish good models from bad. In this paper the relationships between the various criteria are examined for a very general class of models and it is shown that most of the criteria are equivalent. It is also shown how a model can be designed to satisfy these criteria exactly and to be consistent with inertial-subrange theory. Some examples of models that obey the criteria are described. As an illustration some calculations of dispersion in free-convective conditions are presented.

1. Introduction

Stochastic or random-walk models of particle motions have proved to be a successful and flexible tool in the investigation of the dispersion of passive tracers in high-Reynolds-number turbulence (Reid 1979; Wilson, Thurtell & Kidd 1981 *a, c*; Ley 1982; Ley & Thomson 1983; Legg 1983; de Baas, van Dop & Nieuwstadt 1986; Thomson 1986*a*). They are particularly suited to the calculation of dispersion in complex flows, where many other techniques (e.g. similarity theory, Taylor's 1921 statistical theory or eddy-diffusivity techniques) are inappropriate or invalid. They can take account of inhomogeneities, unsteadiness or non-Gaussianity in the turbulent velocity distribution and, unlike eddy-diffusivity methods, can be applied close to a source where the travel time of particles is much less than the Lagrangian timescale. Being Lagrangian in concept, they provide a more natural approach than high-order closure models and, as shown below, are able to represent exactly the advection terms which are parametrized in high-order closure models.

The basis of the approach is to regard the turbulent flow in question as a member of a statistical ensemble of similar flows with identical external conditions (see e.g. Monin & Yaglom 1971, §3.2). To calculate the ensemble mean concentration field, the trajectories of a representative sample of tracer particles, chosen from all tracer particles in the ensemble of flows, are simulated numerically. Provided the Reynolds number is sufficiently large, as for example in the atmosphere, the effect of molecular diffusion on the ensemble mean concentration field is very small (Monin & Yaglom 1971, §10.2); hence molecular diffusion can be neglected and the tracer particles can be assumed to travel at the local velocity of the fluid, i.e. as if they are fluid elements. Because each particle moves independently of the others, these models are called 'one-particle' models.

In most models proposed to date the position and velocity of a fluid element or particle of tracer, considered as a single entity, is assumed to evolve in a Markovian manner. This is a plausible assumption because, in high-Reynolds-number flows, the

Lagrangian acceleration correlation is small over time lags much longer than the Kolmogorov timescale τ_η (Monin & Yaglom 1975, p. 370) and so the changes in a particle's velocity in two successive intervals Δt (where Δt is much larger than τ_η , but small enough that the frequency $1/\Delta t$ lies in the inertial subrange) are nearly independent. Of course they cannot be completely independent or the variance of the particle velocities would grow indefinitely. In making the Markovian assumption it is assumed that this dependence can be accounted for by allowing the velocity increments to depend on the particle's velocity and (in inhomogeneous turbulence) on the position of the particle. A consequence of the Markovian assumption is that the model cannot correctly represent the details of a particle's motion over timescales of order τ_η . Although there is no reason to think the Markovian assumption is exact, it seems reasonable that the acceleration of a particle, with its very short correlation timescale, should have properties that, given the particles' velocity, are determined by local conditions. In contrast the velocity of a particle, with its timescale determined by the largest eddies, is not determined locally and so the position of a particle cannot in general be assumed to be a Markov process.

In inhomogeneous or non-stationary conditions it is not immediately clear how such a model should be formulated. In previous studies many different model formulations have been tried (e.g. Wilson, Thurtell & Kidd 1981*b*; Legg & Raupach 1982; Wilson, Legg & Thomson 1983; Janicke 1983; Ley & Thomson 1983; van Dop, Nieuwstadt & Hunt 1985; de Baas *et al.* 1986; Thomson 1984, 1986*a*) and it has been shown that the results from some models can be seriously in error. A number of different criteria have emerged to distinguish between good and bad models. The four main criteria that have been used are: Does the model give the right steady-state distribution of particles in phase space? (Janicke 1983; Thomson 1984, 1986*a*); Is the small-time behaviour of the velocity distribution of the particles from a point source correct? (van Dop *et al.* 1985); Are the Eulerian equations derived from the model compatible with the true Eulerian equations? (van Dop *et al.* 1985); and Does the model reduce to a diffusion-equation model as the Lagrangian timescale tends to zero? (Durbin 1983, 1984). A further criterion, which has been raised in connection with 'two-particle' models but which is also relevant to one-particle models, is: Are the forward and reverse formulations of the dispersion consistent? (Egbert & Baker 1984).

In this paper the relationships between and the consistency of these criteria are investigated. It is shown that a generalized version of the first condition above is sufficient to ensure that all the other criteria are satisfied and indeed is equivalent to most of them. This condition is not sufficient to determine the formulation of the model uniquely and ways of removing the remaining indeterminacy are discussed. Finally some simple examples of such models are presented.

Although 'two-particle' models are not discussed, many of the ideas presented here are also applicable to such models. Two-particle models can be even more sensitive to the model formulation than one-particle models (Sawford 1983; Thomson 1986*b*) and so their correct formulation is even more important.

In much of the following it is *not* assumed that the density of the fluid is constant. This is done because it enables some insight to be achieved into why most of the criteria are equivalent and because the theory generalizes to variable-density flows quite naturally. Although some of the formulae appear more complex than they would otherwise, this additional complexity is more apparent than real; no real simplifications would be possible by restricting discussion to constant-density flows.

2. Basic assumptions

2.1. Notation

In order to achieve our objective, it is necessary to introduce some notation. $\mathbf{x}(t)$ and $\mathbf{u}(t)$ will be used to denote the position and velocity of a fluid element or particle of tracer at time t . Cartesian components will be denoted by superscripts and the Einstein summation convention will be used. The density function of the phase-space (i.e. (\mathbf{x}, \mathbf{u}) -space) distribution of all the particles of tracer in the ensemble of flows under consideration will be denoted by $g(\mathbf{x}, \mathbf{u}, t)$; the density function of the distribution of the fluid elements will be denoted by $g_a(\mathbf{x}, \mathbf{u}, t)$. Characteristic functions will be denoted by $\hat{}$, e.g.

$$\hat{g}(\mathbf{x}, \boldsymbol{\theta}, t) = \int g(\mathbf{x}, \mathbf{u}, t) \exp(i\mathbf{u} \cdot \boldsymbol{\theta}) d^3\mathbf{u}.$$

$\mathbf{u}_E(\mathbf{x}, t)$, $\rho(\mathbf{x}, t)$ and $c(\mathbf{x}, t)$ will be used to denote the Eulerian velocity, density and concentration fields respectively in a particular realization of the flow and the ensemble average of an Eulerian quantity will be indicated by angled brackets, $\langle \rangle$. g and g_a will be normalized so that

$$\int g d^3\mathbf{u} = \hat{g}(\mathbf{x}, 0, t) = \langle c(\mathbf{x}, t) \rangle \quad \text{and} \quad \int g_a d^3\mathbf{u} = \hat{g}_a(\mathbf{x}, 0, t) = \langle \rho(\mathbf{x}, t) \rangle.$$

This normalization has an advantage over the normalization

$$\int g d^3\mathbf{u} d^3\mathbf{x} = \int g_a d^3\mathbf{u} d^3\mathbf{x} = 1$$

in that it can be applied in unbounded flows; however it means that g and g_a are not strictly *probability* density functions in phase space. It can easily be seen that, for any function $f(\mathbf{x}, \mathbf{u}, t)$, $\int gf d^3\mathbf{u}$ equals $\langle c(\mathbf{x}, t) \rangle$ times the average value of f for particles of tracer at \mathbf{x} . This average value is equal to the concentration-weighted Eulerian average value $\langle cf(\mathbf{x}, \mathbf{u}_E, t) \rangle / \langle c \rangle$ (this is essentially the result derived by van Dop *et al.* 1985, Appendix A). Hence $\int gf d^3\mathbf{u} = \langle cf(\mathbf{x}, \mathbf{u}_E, t) \rangle$ and, similarly, $\int g_a f d^3\mathbf{u} = \langle \rho f(\mathbf{x}, \mathbf{u}_E, t) \rangle$. In particular

$$\hat{g} = \langle c \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \rangle \quad \text{and} \quad \hat{g}_a = \langle \rho \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \rangle.$$

$g_a(\mathbf{x}, \mathbf{u}, t) / \langle \rho(\mathbf{x}, t) \rangle$ is the density-weighted probability density function (p.d.f.) of the Eulerian velocity at (\mathbf{x}, t) . We will call the turbulence Gaussian if g_a has the form

$$g_a = \frac{\langle \rho \rangle}{(2\pi)^{\frac{3}{2}} (\det V)^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{u}^i - U^i)(V^{-1})^{ij}(\mathbf{u}^j - U^j)\right)$$

for some $U(\mathbf{x}, t)$ and $V(\mathbf{x}, t)$. It can easily be seen that $U = \langle \rho \mathbf{u}_E \rangle / \langle \rho \rangle$ and $V^{ij} = \langle \rho(u_E^i - U^i)(u_E^j - U^j) \rangle / \langle \rho \rangle$. U and V will be used to stand for these quantities even in non-Gaussian turbulence. An overbar will be used to denote an average over all particles of tracer in the ensemble of flows.

2.2. Statistical theory

Consider a particular realization ω of the flow and consider the fluid element which is at position \mathbf{y} at time s . Let $p^\omega(\mathbf{x}, t | \mathbf{y}, s)$ be the p.d.f. of the position of the fluid element at time t (since we are neglecting molecular diffusion this will be a delta

function). If the source strength in this realization is $S^\omega(\mathbf{x}, t)$ then, because the tracer particles move as if they are fluid elements, the concentration of tracer at time t is

$$c(\mathbf{x}, t) = \int_{s < t} p^\omega(\mathbf{x}, t | \mathbf{y}, s) S^\omega(\mathbf{y}, s) d^3\mathbf{y} ds. \quad (1)$$

Now suppose the source strength in each member of the ensemble is proportional to ρ (i.e. $S^\omega(\mathbf{x}, t) = S(\mathbf{x}, t) \rho(\mathbf{x}, t) / \langle \rho(\mathbf{x}, t) \rangle$, S being the same in each realization) so that the source simply 'marks' a certain fraction of the fluid elements passing by. Taking the ensemble average of (1) yields

$$\langle c(\mathbf{x}, t) \rangle = \int_{s < t} p(\mathbf{x}, t | \mathbf{y}, s) S(\mathbf{y}, s) d^3\mathbf{y} ds,$$

where $p(\mathbf{x}, t | \mathbf{y}, s) d^3\mathbf{x} = \langle p^\omega(\mathbf{x}, t | \mathbf{y}, s) \rho(\mathbf{y}, s) \rangle d^3\mathbf{x} / \langle \rho(\mathbf{y}, s) \rangle$ is the probability that a fluid element (chosen at random from all the fluid elements in the ensemble of flows) is, at time t , in the elemental volume $d^3\mathbf{x}$ centred on \mathbf{x} given that it is at position \mathbf{y} at time s (the fluid element is more likely to come from a realization where $\rho(\mathbf{y}, s)$ is large than from one where it is small).

Similar results hold in phase space. Again consider the fluid element that is at position \mathbf{y} at time s in a particular realization ω of the flow and let $p^\omega(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, s)$ be the p.d.f. of the position and velocity of the fluid element at time t . Then the concentration of tracer in phase space in the realization ω is

$$\int_{s < t} p^\omega(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, s) S^\omega(\mathbf{y}, s) d^3\mathbf{y} ds. \quad (2)$$

In the phase-space calculation we can consider sources whose strength depends on the velocity at the source (e.g. a conditional release, that is a source that switches on when the velocity at the source satisfies certain constraints). Suppose $S^\omega(\mathbf{x}, t) = S(\mathbf{x}, \mathbf{u}_E(\mathbf{x}, t), t) \rho(\mathbf{x}, t) / \langle \rho(\mathbf{x}, t) \rangle$ and let $\langle \rangle_v$ denote an average over the subensemble of realizations in which $\mathbf{u}_E(\mathbf{y}, s) = \mathbf{v}$. Then

$$\langle p^\omega(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, s) S^\omega(\mathbf{y}, s) \rangle_v = \frac{p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s) \langle \rho(\mathbf{y}, s) \rangle_v S(\mathbf{y}, \mathbf{v}, s)}{\langle \rho(\mathbf{y}, s) \rangle}, \quad (3)$$

where

$$p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s) d^3\mathbf{x} d^3\mathbf{u} = \langle p^\omega(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, s) \rho(\mathbf{y}, s) \rangle_v d^3\mathbf{x} d^3\mathbf{u} / \langle \rho(\mathbf{y}, s) \rangle_v$$

is the probability that a fluid element, chosen at random from all the fluid elements in the ensemble of flows, is, at time t , in the elemental volume $d^3\mathbf{x} d^3\mathbf{u}$ of phase space centred on (\mathbf{x}, \mathbf{u}) given that it is at (\mathbf{y}, \mathbf{v}) at time s . Averaging (3) over the whole ensemble yields

$$\begin{aligned} \langle p^\omega(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, s) S^\omega(\mathbf{y}, s) \rangle &= \frac{\langle p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{u}_E(\mathbf{y}, s), s) \rho(\mathbf{y}, s) S(\mathbf{y}, \mathbf{u}_E(\mathbf{y}, s), s) \rangle}{\langle \rho(\mathbf{y}, s) \rangle} \\ &= \int p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s) \frac{g_a(\mathbf{y}, \mathbf{v}, s)}{\langle \rho(\mathbf{y}, s) \rangle} S(\mathbf{y}, \mathbf{v}, s) d^3\mathbf{v}. \end{aligned}$$

Hence the ensemble average of (2) is

$$g(\mathbf{x}, \mathbf{u}, t) = \int_{s < t} p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s) \frac{g_a(\mathbf{y}, \mathbf{v}, s)}{\langle \rho(\mathbf{y}, s) \rangle} S(\mathbf{y}, \mathbf{v}, s) d^3\mathbf{v} d^3\mathbf{y} ds.$$

This equation indicates how the phase-space density of tracer particles, g , is related to the source of particles in phase space, $g_a S / \langle \rho \rangle$, by the transition probability density $p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s)$.

2.3. Markovian stochastic models

As indicated in the Introduction we shall consider models in which, for a fluid element chosen at random from all the fluid elements in the ensemble of flows, the evolution of (\mathbf{x}, \mathbf{u}) is a Markov process. The mathematics of Markov processes is well understood and several standard results concerning such processes are quoted below. These results can be found in e.g. Arnold (1974), Gihman & Skorohod (1974, 1975, 1979) or Schuss (1980). Let us also assume that \mathbf{x} and \mathbf{u} are continuous functions of t with $d\mathbf{x}/dt = \mathbf{u}$ and that the process satisfies a mild regularity condition, namely that it has the same local structure as a process with independent increments. With these assumptions the evolution of (\mathbf{x}, \mathbf{u}) can be described by the stochastic differential equations

$$d\mathbf{u}^i = a^i(\mathbf{x}, \mathbf{u}, t) dt + b^{ij}(\mathbf{x}, \mathbf{u}, t) d\xi^j, \tag{4a}$$

$$d\mathbf{x} = \mathbf{u} dt, \tag{4b}$$

where \mathbf{a} and \mathbf{b} are functions of \mathbf{x} , \mathbf{u} and t and the $d\xi^i$ are the increments of a vector-valued Wiener process with independent components (see Appendix A). The increments $d\xi^i$ are Gaussian with mean zero and variance dt ; increments $d\xi^i$ and $d\xi^j$ occurring at different times, or at the same time with $i \neq j$, are independent. B^{ij} will be used to denote $\frac{1}{2}b^{ik}b^{jk}$. Although \mathbf{B} does not determine \mathbf{b} , it does determine the distribution of the random increments $b^{ij} d\xi^j$; hence the specification of \mathbf{a} and \mathbf{B} is sufficient to determine the way the particles move. A sample of the trajectories can be calculated numerically by replacing the infinitesimal increments $d\mathbf{u}$, $d\mathbf{x}$, dt and $d\xi$ by finite increments $\Delta\mathbf{u}$, $\Delta\mathbf{x}$, Δt and $\Delta\xi$.

It is of interest that the random increments in (4) must be Gaussian (see Appendix A). This has implications for a previously proposed model (Thomson 1984) which requires non-Gaussian forcing in order to satisfy the criteria mentioned in the Introduction. Such a model must either be non-existent (in the sense that no random forcing exists with the required moments) or have discontinuous phase-space trajectories. In many cases it is the former that is the case. For example consider inhomogeneous Gaussian turbulence in one dimension with no mean flow. The model in question (Thomson 1984, §3) requires the first three moments of the random increments to be $O(dt)$ with higher moments $O(dt^2)$. Now any random variable X must satisfy $(\overline{X^3})^2 \leq \overline{X^2} \overline{X^4}$ (Feller 1966, p. 151). Hence there is no random forcing with the required moments. In some non-Gaussian cases the situation can be even worse with the model requiring increments with negative variance (de Baas *et al.* 1986). Of course for a particular finite value of Δt it may be possible to choose the distribution of the random increments in order to satisfy the criteria at least approximately. The model has been used successfully in this way by a number of authors (e.g. Thomson 1984; de Baas *et al.* 1986). However such a model is difficult to analyse and is rather unsatisfactory mathematically because the length of the time step Δt plays an essential role and the well-mixed condition is normally only satisfied approximately.

In manipulating (4) it must be remembered that $(d\xi^i)^2$ is of order dt and so cannot be neglected in comparison with dt . A consequence of this is that the derivative of a given function of the position and velocity of a particle is not given by the usual 'function of a function' rule, but by Itô's formula

$$d(f(\mathbf{x}, \mathbf{u}, t)) = \left(\frac{\partial f}{\partial t} + u^i \frac{\partial f}{\partial x^i} + a^i \frac{\partial f}{\partial u^i} + B^{ij} \frac{\partial^2 f}{\partial u^i \partial u^j} \right) dt + \frac{\partial f}{\partial u^i} b^{ij} d\xi^j.$$

Equation (4) implies that, away from any sources, g satisfies

$$\frac{\partial g}{\partial t} = -\frac{\partial}{\partial x^i}(u^i g) - \frac{\partial}{\partial u^i}(a^i(\mathbf{x}, \mathbf{u}, t)g) + \frac{\partial^2}{\partial u^i \partial u^j}(B^{ij}(\mathbf{x}, \mathbf{u}, t)g). \quad (5)$$

This is called the forward Kolmogorov or Fokker–Plank equation for the system (4). Equation (5) shows that the flux of tracer in the x^i direction, $u^i g$, and that in the u^i direction, $a^i g - \partial(B^{ij}g)/\partial u^j$, together balance the rate of change of the phase-space density g . Equation (5) is, of course, also satisfied by $p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s)$ for $t > s$. $p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s)$ also satisfies the backward Kolmogorov equation

$$\frac{\partial p}{\partial s} = -v^i \frac{\partial p}{\partial y^i} - a^i(\mathbf{y}, \mathbf{v}, s) \frac{\partial p}{\partial v^i} - B^{ij}(\mathbf{y}, \mathbf{v}, s) \frac{\partial^2 p}{\partial v^i \partial v^j}, \quad (6)$$

for $t > s$.

Equation (5) can be written in the form

$$\frac{\partial g}{\partial t} = -\frac{\partial}{\partial x^i}(u^i g) + \psi_x(g), \quad (7)$$

where, for fixed \mathbf{x} , ψ_x is an operator that maps g (considered as a function of \mathbf{u}) to a new function $\psi_x(g)$ of \mathbf{u} . For many of the arguments in §3 below it is only assumed that the evolution equation for g has the form (7) and that the particles in the model move independently (which implies that ψ_x is a linear operator). A consequence of this is that many of the results in §3 are applicable to more general models than (4), such as the models with skew forcing discussed above (when they exist) and the model of Smith (1984). In Smith's model the particle velocities do not change continuously but in discrete jumps which occur at random times. In terms of characteristic functions, (7) can be expressed as

$$\frac{\partial \hat{g}}{\partial t} = i \frac{\partial^2 \hat{g}}{\partial x^i \partial \theta^i} + \psi_x(\hat{g}), \quad (8)$$

where ψ_x maps \hat{g} to $\int \psi_x(g) \exp(i\mathbf{u} \cdot \boldsymbol{\theta}) d^3\mathbf{u}$.

For the arguments that follow it is necessary to make a mild assumption about the behaviour of g and g_a as $|\mathbf{u}| \rightarrow \infty$. Consider an expression consisting of g , g_a or a derivative of g or g_a , multiplied by a number of terms, each term being a component of \mathbf{u} , \mathbf{a} , \mathbf{B} or a derivative of \mathbf{a} or \mathbf{B} . It is assumed that g and g_a tend to zero sufficiently rapidly as $|\mathbf{u}| \rightarrow \infty$ so that the integral of the expression over \mathbf{u} -space exists.

3. Five criteria for the selection of stochastic models of particle trajectories

3.1. The well-mixed condition

The first criterion that will be discussed is the following: If the particles of tracer are initially well-mixed (i.e. g proportional to g_a) will they remain so? This is a generalized form of the steady-state criterion mentioned in the Introduction and is, unlike the steady-state criterion, applicable to non-stationary situations. It will be referred to as the well-mixed condition.

For the model (4) to satisfy the well-mixed condition it is necessary and sufficient that $g = g_a$ should satisfy (5). This leads to the condition

$$a^i g_a = \frac{\partial}{\partial u^j}(B^{ij}g_a) + \phi^i(\mathbf{x}, \mathbf{u}, t), \quad (9a)$$

where ϕ satisfies

$$\frac{\partial \phi^i}{\partial u^i} = -\frac{\partial g_a}{\partial t} - \frac{\partial}{\partial x^i} (u^i g_a). \tag{9b}$$

From (9a) and the assumed behaviour of g_a as $|\mathbf{u}| \rightarrow \infty$ it follows that the integral over \mathbf{u} -space of a component of ϕ times components of \mathbf{u} , \mathbf{a} , \mathbf{B} and their derivatives must exist. In particular

$$\phi \rightarrow 0 \quad \text{as } |\mathbf{u}| \rightarrow \infty. \tag{10}$$

In terms of ψ , the well-mixed condition can be expressed as

$$\frac{\partial \hat{g}_a}{\partial t} = i \frac{\partial^2 \hat{g}_a}{\partial x^i \partial \theta^i} + \psi_x(\hat{g}_a). \tag{11}$$

3.2. The small-time behaviour of the velocity distribution of particles from a point source

Consider now the behaviour of the velocity distribution of particles from an instantaneous point source at (\mathbf{x}_s, t_s) . The source strength will be assumed proportional to $\rho(\mathbf{x}_s, t_s)$, i.e. the source simply marks the fluid elements as they pass through (\mathbf{x}_s, t_s) . The density function of the velocity distribution of these particles will be denoted by $h(\mathbf{u}, t)$. In terms of g ,

$$h(\mathbf{u}, t) = \int g(\mathbf{x}, \mathbf{u}, t) d^3\mathbf{x} \Big/ \int \langle c(\mathbf{x}, t) \rangle d^3\mathbf{x}.$$

Integrating (8) and noting that $\int \langle c(\mathbf{x}, t) \rangle d^3\mathbf{x}$ is independent of t yields

$$\frac{\partial \hat{h}}{\partial t} = \frac{\int \psi_x(\hat{g}) d^3\mathbf{x}}{\int \langle c \rangle d^3\mathbf{x}}.$$

At $t = t_s$, \hat{g} is zero except at $\mathbf{x} = \mathbf{x}_s$ and so ψ_x can be replaced by $\hat{\psi}_{x_s}$. Hence, using the linearity of $\hat{\psi}_{x_s}$,

$$\left(\frac{\partial \hat{h}}{\partial t} \right)_{t_s} = \hat{\psi}_{x_s}(\hat{h}(\boldsymbol{\theta}, t_s)),$$

the subscript t_s indicating that $\partial \hat{h} / \partial t$ is evaluated at time t_s . Initially h is identical with the velocity distribution of the fluid elements at the source and so

$$\hat{h}(\boldsymbol{\theta}, t_s) = \hat{g}_a(\mathbf{x}_s, \boldsymbol{\theta}, t_s) / \langle \rho(\mathbf{x}_s, t_s) \rangle.$$

Hence, using again the linearity of $\hat{\psi}_{x_s}$,

$$\left(\frac{\partial \hat{h}}{\partial t} \right)_{t_s} = \frac{1}{\langle \rho(\mathbf{x}_s, t_s) \rangle} \hat{\psi}_{x_s}(\hat{g}_a(\mathbf{x}_s, \boldsymbol{\theta}, t_s)). \tag{12}$$

At small times however we know the true behaviour of the particle velocities:

$$\left(\frac{d\mathbf{u}}{dt} \right)_{t_s} = \left(\frac{\partial \mathbf{u}_E}{\partial t} + \mathbf{u}_E \cdot \nabla \mathbf{u}_E \right)_{(\mathbf{x}_s, t_s)}. \tag{13}$$

Hence we can calculate the true evolution of \hat{h} . By definition $\hat{h} = \overline{\exp(i\mathbf{u} \cdot \boldsymbol{\theta})}$ and so

$$\frac{\partial \hat{h}}{\partial t} = i\boldsymbol{\theta} \cdot \overline{\frac{d\mathbf{u}}{dt}} \exp(i\mathbf{u} \cdot \boldsymbol{\theta}).$$

Now the number of particles of tracer in a particular flow realization is proportional to $\rho(\mathbf{x}_s, t_s)$. Hence, using (13)

$$\left(\frac{\partial \hat{h}}{\partial t}\right)_{t_s} = \frac{i\theta}{\langle \rho(\mathbf{x}_s, t_s) \rangle} \cdot \left\langle \rho \left(\frac{\partial \mathbf{u}_E}{\partial t} + \mathbf{u}_E \cdot \nabla \mathbf{u}_E \right) \exp(i\mathbf{u}_E \cdot \theta) \right\rangle_{(\mathbf{x}_s, t_s)}.$$

Applying continuity, $\partial \rho / \partial t + \nabla \cdot (\rho \mathbf{u}_E) = 0$, yields

$$\begin{aligned} \left(\frac{\partial \hat{h}}{\partial t}\right)_{t_s} &= \frac{1}{\langle \rho(\mathbf{x}_s, t_s) \rangle} \left(\left(\frac{\partial}{\partial t} - i \frac{\partial^2}{\partial x^i \partial \theta^i} \right) \langle \rho \exp(i\mathbf{u}_E \cdot \theta) \rangle \right)_{(\mathbf{x}_s, t_s)} \\ &= \frac{1}{\langle \rho(\mathbf{x}_s, t_s) \rangle} \left(\frac{\partial \hat{g}_a}{\partial t} - i \frac{\partial^2 \hat{g}_a}{\partial x^i \partial \theta^i} \right)_{(\mathbf{x}_s, t_s)}. \end{aligned} \quad (14)$$

Equations (12) and (14) show that for the velocity distribution of particles from a point source to behave correctly at small times, it is necessary and sufficient that

$$\frac{\partial \hat{g}_a}{\partial t} = i \frac{\partial^2 \hat{g}_a}{\partial x^i \partial \theta^i} + \psi_x(\hat{g}_a)$$

at the source. Hence we see that requiring the correct small-time behaviour of the velocity distribution of particles from a point source is equivalent to the well-mixed condition (11).

3.3. The requirement of compatibility with the Eulerian equations

In this section, (8) is compared with the true evolution equation for g derived from the Eulerian equations. Neglecting molecular diffusion, the Eulerian equations take the form

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}_E c) = 0, \quad (15a)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{u}_E \rho) = 0, \quad (15b)$$

$$\frac{\partial \mathbf{u}_E}{\partial t} + \mathbf{u}_E \cdot \nabla \mathbf{u}_E = \frac{D\mathbf{u}_E}{Dt}, \quad (15c)$$

where $D\mathbf{u}_E/Dt$, the acceleration of a fluid element, is the result of the pressure, viscous and external forces (e.g. gravity). (Note no specific form for $D\mathbf{u}_E/Dt$ is assumed. Of course if a form for $D\mathbf{u}_E/Dt$ were assumed, the resulting equations would contain much more information about the flow but would also be, as is well known, very intractable.)

Equations (15) give rise to an infinite sequence of equations for the evolution of the moments $\langle c u_E^i \dots u_E^m \rangle$, $\langle \rho u_E^i \dots u_E^m \rangle$. By using characteristic functions this infinite hierarchy can be expressed more conveniently in two equations. To derive these equations we note that (15) implies

$$\begin{aligned} \left(\frac{\partial}{\partial t} - i \frac{\partial^2}{\partial x^i \partial \theta^i} \right) (c \exp(i\mathbf{u}_E \cdot \theta)) &= i c \exp(i\mathbf{u}_E \cdot \theta) \theta \cdot \frac{D\mathbf{u}_E}{Dt}, \\ \left(\frac{\partial}{\partial t} - i \frac{\partial^2}{\partial x^i \partial \theta^i} \right) (\rho \exp(i\mathbf{u}_E \cdot \theta)) &= i \rho \exp(i\mathbf{u}_E \cdot \theta) \theta \cdot \frac{D\mathbf{u}_E}{Dt}, \end{aligned}$$

which, on taking the ensemble average, yields

$$\left(\frac{\partial}{\partial t} - i \frac{\partial^2}{\partial x^i \partial \theta^i}\right) \hat{g} = i \left\langle c \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \boldsymbol{\theta} \cdot \frac{D\mathbf{u}_E}{Dt} \right\rangle, \tag{16a}$$

$$\left(\frac{\partial}{\partial t} - i \frac{\partial^2}{\partial x^i \partial \theta^i}\right) \hat{g}_a = i \left\langle \rho \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \boldsymbol{\theta} \cdot \frac{D\mathbf{u}_E}{Dt} \right\rangle. \tag{16b}$$

Unfortunately no stochastic model of particle motions can produce the evolution equation (16a) exactly because (16a) contains terms involving $D\mathbf{u}_E/Dt$ which cannot be determined from \hat{g} and \hat{g}_a . However it can produce an evolution equation of the same form as (16a) with the right-hand side of (16a) being parametrized in terms of \hat{g} and \hat{g}_a . Comparing (8) and (16a), it can be seen that the parametrization is

$$i \left\langle c \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \boldsymbol{\theta} \cdot \frac{D\mathbf{u}_E}{Dt} \right\rangle = \hat{\psi}_x(\hat{g}).$$

There is only one obvious constraint which (16) imposes on the parametrization, although the possibility of other more subtle constraints cannot be ruled out (to be completely consistent with (16) there must exist an ensemble of velocity and density fields satisfying (15b) for which the model (4) is exact – see §3.6 below). If $c = \rho$ in each realization then $\hat{g} = \hat{g}_a$ and the right-hand side of (16a) equals the left-hand side of (16b). If the parametrization of the right-hand side of (16a) is also to have this property, then

$$\left(\frac{\partial}{\partial t} - i \frac{\partial^2}{\partial x^i \partial \theta^i}\right) \hat{g}_a = \hat{\psi}_x(\hat{g}_a) \tag{17}$$

must be satisfied. This is simply the well-mixed condition. If we regard the model as being ‘compatible’ with the Eulerian equations whenever the parametrization satisfies (17), then the model is compatible with the Eulerian equations if and only if the well-mixed condition is satisfied.

Of course, out of all conceivable parametrizations of the right-hand side of (16a) which satisfy (17), only a small fraction are physically reasonable. It seems likely however that a physically plausible model for the particle trajectories will correspond to a physically reasonable parametrization. Some examples are discussed in §5 below. It is of interest to note that a model of the form (4) contains less parametrization than a high-order closure model; high-order closure models require, in addition to the parametrization of the $D\mathbf{u}_E/Dt$ terms, the parametrization of some quantities of the form $\langle c u_E^i \dots u_E^m \rangle$ that occur in the advection terms.

From (5) and (16a) it can be seen that in terms of \mathbf{a} and \mathbf{B} the parametrization is

$$\begin{aligned} i \left\langle c \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \boldsymbol{\theta} \cdot \frac{D\mathbf{u}_E}{Dt} \right\rangle &= \int \left(-\frac{\partial}{\partial u^i} (a^i g) + \frac{\partial^2}{\partial u^i \partial u^j} (B^{ij} g) \right) e^{i\mathbf{u} \cdot \boldsymbol{\theta}} d^3\mathbf{u} \\ &= i\theta^i \langle a^i(\mathbf{x}, \mathbf{u}_E, t) c \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \rangle - \theta^i \theta^j \langle B^{ij}(\mathbf{x}, \mathbf{u}_E, t) c \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \rangle. \end{aligned} \tag{18}$$

By noting that $i \langle c \exp(i\mathbf{u}_E \cdot \boldsymbol{\theta}) \boldsymbol{\theta} \cdot D\mathbf{u}_E/Dt \rangle$ is equal to $\langle c \rangle$ times the average value of $d \exp(i\mathbf{u}(t) \cdot \boldsymbol{\theta})/dt$ for particles of tracer at \mathbf{x} , Itô’s formula can be used to derive

(18) directly. Neglecting variations in ρ , the first two moments of this parametrization are given by

$$\left\langle c \left(\frac{Du_{\mathbf{E}}^i}{Dt} \right) \right\rangle = \langle ca^i(\mathbf{u}_{\mathbf{E}}) \rangle,$$

$$\left\langle c \left(u_{\mathbf{E}}^i \left(\frac{Du_{\mathbf{E}}^j}{Dt} \right) + u_{\mathbf{E}}^j \left(\frac{Du_{\mathbf{E}}^i}{Dt} \right) \right) \right\rangle = \langle c(u_{\mathbf{E}}^i a^j(\mathbf{u}_{\mathbf{E}}) + u_{\mathbf{E}}^j a^i(\mathbf{u}_{\mathbf{E}})) \rangle + 2\langle cB^{ij}(\mathbf{u}_{\mathbf{E}}) \rangle.$$

Using the well-mixed condition this can be expressed as

$$\left\langle c' \left(\frac{Du_{\mathbf{E}}^i}{Dt} \right)' \right\rangle = \langle c' a^i \rangle,$$

$$\left\langle c' \left(u_{\mathbf{E}}^i \left(\frac{Du_{\mathbf{E}}^j}{Dt} \right)' + u_{\mathbf{E}}^j \left(\frac{Du_{\mathbf{E}}^i}{Dt} \right)' \right) \right\rangle = \langle c'(u_{\mathbf{E}}^i a^j + u_{\mathbf{E}}^j a^i) \rangle + 2\langle c' B^{ij} \rangle,$$

where a prime denotes the departure of a quantity from its ensemble average. Some examples are given in §5.

3.4. Forward and reverse diffusion

Consider a fluid element chosen at random from all the fluid elements in the ensemble of flows. Let A_1 be the event 'at time t the fluid element lies in the phase-space volume $d^3\mathbf{x} d^3\mathbf{u}$ centred on (\mathbf{x}, \mathbf{u}) ' and let A_2 be the event 'at time s the fluid element lies in the volume $d^3\mathbf{y} d^3\mathbf{v}$ centred on (\mathbf{y}, \mathbf{v}) '. The probability of A_1 and A_2 both occurring is equal to the probability of A_1 given A_2 (i.e. $p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s) d^3\mathbf{x} d^3\mathbf{u}$) times the probability of A_2 occurring (i.e. $g_a(\mathbf{y}, \mathbf{v}, s) d^3\mathbf{y} d^3\mathbf{v} / \int g_a(\mathbf{z}, \mathbf{w}, s) d^3\mathbf{z} d^3\mathbf{w}$). By also evaluating this with A_1 and A_2 reversed and equating the two expressions we obtain

$$p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s) g_a(\mathbf{y}, \mathbf{v}, s) = p(\mathbf{y}, \mathbf{v}, s | \mathbf{x}, \mathbf{u}, t) g_a(\mathbf{x}, \mathbf{u}, t). \quad (19)$$

(If $\int g_a(\mathbf{z}, \mathbf{w}, s) d^3\mathbf{z} d^3\mathbf{w}$, the total mass of fluid, is infinite the above argument fails but (19) can still be obtained from the obvious limiting argument.) Assuming $t > s$, this relates the forward transition probability density $p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s)$ to the reverse transition density $p(\mathbf{y}, \mathbf{v}, s | \mathbf{x}, \mathbf{u}, t)$. By either integrating (19) with respect to \mathbf{u} and \mathbf{v} or by a direct argument analogous to that used to derive (19), we obtain

$$p(\mathbf{x}, t | \mathbf{y}, s) \langle \rho(\mathbf{y}, s) \rangle = p(\mathbf{y}, s | \mathbf{x}, t) \langle \rho(\mathbf{x}, t) \rangle.$$

If ρ is constant, this is the condition discussed by Egbert & Baker (1984) in the context of two-particle models.

For $t > s$, $p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s)$ can be calculated from the model (4) (it is simply the p.d.f. of the distribution of fluid elements that commence at (\mathbf{y}, \mathbf{v}) at time s). $p(\mathbf{y}, \mathbf{v}, s | \mathbf{x}, \mathbf{u}, t)$ could also be calculated (in principle) from the model by considering all trajectories resulting from a well-mixed distribution of particles (i.e. a distribution with density function proportional to g_a) at time s and then noting the position and velocity at time s of those trajectories that pass through (\mathbf{x}, \mathbf{u}) at time t . It seems reasonable to propose that the value of p obtained should satisfy (19) if the model is to be acceptable. In fact it is easy to see that this is equivalent to the well-mixed condition. Suppose the well-mixed condition is satisfied and consider all model trajectories resulting from a well-mixed distribution of particles at time s . Then the argument leading to (19) applies equally well to the model trajectories and so (19) is satisfied. Conversely if (19) is satisfied, the integral of the left-hand side of (19) with respect to \mathbf{y} and \mathbf{v} is proportional to the phase-space density of tracer at time t

resulting from a well-mixed distribution at time s , and the integral of the right-hand side is equal to $g_a(\mathbf{x}, \mathbf{u}, t)$. Hence the well-mixed condition is satisfied.

It is of some interest to see if there is a way of calculating $p(\mathbf{y}, \mathbf{v}, s | \mathbf{x}, \mathbf{u}, t)$, $t > s$, from the model that is simpler than that given above. For example, if one is only interested in $\langle c \rangle$ at a particular point resulting from an extended source, it is wasteful to calculate many forward trajectories, only a few of which will pass through the point. The obvious approach is to try to simulate the motion of particles backwards in time. That this is not completely straightforward can be seen by considering two situations with different values of g_a at $t = 0$ in which all the fluid elements move according to the same stochastic differential equations; the stochastic differential equations describing the backward trajectories will be different in the two cases.

Let us set $t' = -t$ and $\mathbf{u}' = -\mathbf{u}$ (for this section only) so that t' increases as we go back in time and denote the stochastic differential equation that we hope will describe the backwards trajectories by

$$d\mathbf{u}' = \mathbf{a}' dt' + \mathbf{b}'^{ij} d\xi^j, \tag{20a}$$

$$d\mathbf{x} = \mathbf{u}' dt'. \tag{20b}$$

To simplify the notation let $\tilde{a}^i(\mathbf{x}, \mathbf{u}, t) = (1/g_a) \partial(B^{ij}g_a)/\partial u^j$. Using (6), (9) and (19) it can be seen that $p(\mathbf{y}, \mathbf{v}, s | \mathbf{x}, \mathbf{u}, t)$ satisfies

$$\frac{\partial p}{\partial s} = -\frac{\partial}{\partial y^i}(v^i p) - \frac{\partial}{\partial v^i} \left(\left(\frac{\phi^i}{g_a} - \tilde{a}^i \right) p \right) - \frac{\partial^2}{\partial v^i \partial v^j} (B^{ij} p),$$

for $t > s$, where ϕ , g_a , \tilde{a} and \mathbf{B} are evaluated at $(\mathbf{y}, \mathbf{v}, s)$. The forward transition density for our model (20) will be denoted by $p'(\mathbf{x}, \mathbf{u}', t' | \mathbf{y}, \mathbf{v}', s')$, $t' > s'$. We want this to equal the reverse transition density $p(\mathbf{x}, \mathbf{u}, t | \mathbf{y}, \mathbf{v}, s)$, $s > t$, evaluated at $\mathbf{u} = -\mathbf{u}'$, $\mathbf{v} = -\mathbf{v}'$, $t = -t'$, $s = -s'$. Hence $p'(\mathbf{x}, \mathbf{u}', t' | \mathbf{y}, \mathbf{v}', s')$ should satisfy

$$\frac{\partial p'}{\partial t'} = -\frac{\partial}{\partial x^i}(u'^i p') - \frac{\partial}{\partial u'^i} \left(\left(\frac{\phi^i}{g_a} - \tilde{a}^i \right) p' \right) + \frac{\partial^2}{\partial u'^i \partial u'^j} (B^{ij} p')$$

for $t' > s'$, where ϕ , g_a , \tilde{a} and \mathbf{B} are evaluated at $(\mathbf{x}, -\mathbf{u}', -t')$. If the model (20) is to give rise to this forward Kolmogorov equation then we must have

$$\mathbf{a}' = -\tilde{\mathbf{a}} + \frac{\phi}{g_a}, \quad \mathbf{b}' = \mathbf{b},$$

with ϕ , g_a , $\tilde{\mathbf{a}}$ and \mathbf{b} evaluated at $(\mathbf{x}, -\mathbf{u}', -t')$. Note the two parts of \mathbf{a} transform differently under time reversal.

3.5. The small-timescale limit

Durbin (1983, 1984) posed the requirement that a random-walk model should reduce to a diffusion-equation model as the Lagrangian timescale τ tends to zero. In this section we investigate the relation of this requirement to the well-mixed condition.

Suppose the shortest time after the release of material at which we are interested in the dispersion is T and that the timescale on which conditions change as viewed by a particle (due to inhomogeneity or unsteadiness in the turbulence) is τ_H . Let us choose our unit of time so that $\min(T, \tau_H)$ is of order unity and assume that τ is small compared with unity. Our unit of length is chosen so that the size of a cloud of tracer from a point source is of order unity at times of order unity after release. In this coordinate system the turbulent energy must be large to make up for the small

timescale and so we put $g_a = \epsilon^3 f(\mathbf{x}, \mathbf{v}, t)$ where $\mathbf{v} = \epsilon(\mathbf{u} - \mathbf{U})$ and ϵ is a small parameter. It is not yet clear how \mathbf{a} and \mathbf{B} are related to the Lagrangian timescale. However, because the particle velocities are large and rapidly changing, it is clear that \mathbf{B} must be large. In anticipation of the result we put $\mathbf{B} = \beta/\epsilon^4$ and assume that ϕ is of order unity or smaller; if \mathbf{B} is not of order ϵ^{-4} or ϕ is larger than ϵ^0 it can be shown, by repeating the analysis below with different assumptions about the size of \mathbf{B} and ϕ , that the dispersion is not of order unity at times of order unity. Of course ϕ needs to be no larger than $O(\epsilon)$ in order to satisfy (9b) and in one-dimensional models it cannot be larger than this. The scaling for \mathbf{B} can be made plausible by considering diffusion in one dimension in homogeneous stationary Gaussian turbulence. Equation (4) can then take the form of the Langevin equation (see §5) for which the diffusivity at times $t \gg \tau$ equals σ^4/B , σ^2 being the one-dimensional equivalent of V^{ij} . ϵ has been defined so that $\sigma^2 = O(\epsilon^{-2})$ and so B must be of order ϵ^{-4} if the diffusivity is to be of order unity.

Assuming the model satisfies the well-mixed condition, (5) and (9) yield

$$\frac{\partial g}{\partial t} = -\left(\frac{v^i}{\epsilon} + U^i\right)\left(\frac{\partial g}{\partial x^i} - \epsilon \frac{\partial g}{\partial v^j} \frac{\partial U^j}{\partial x^i}\right) + \frac{1}{\epsilon^2} \frac{\partial}{\partial v^i} \left(\beta^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g}{f} \right) \right) - \frac{1}{\epsilon^2} \frac{\partial}{\partial v^i} \left(\frac{\phi^i g}{f} \right), \quad (21)$$

with ϕ satisfying

$$\frac{\partial \phi^i}{\partial v^i} = -\epsilon v^i \frac{\partial f}{\partial x^i} - \epsilon^2 \frac{\partial f}{\partial t} - \epsilon^2 U^i \frac{\partial f}{\partial x^i} + \epsilon^2 v^i \frac{\partial f}{\partial v^j} \frac{\partial U^j}{\partial x^i} + \epsilon^3 \frac{\partial f}{\partial v^i} \left(\frac{\partial U^i}{\partial t} + U^j \frac{\partial U^i}{\partial x^j} \right).$$

From §3.1 it is clear that $\phi \rightarrow 0$ faster than any power of $|\mathbf{v}|$ as $|\mathbf{v}| \rightarrow \infty$. Because there is no flux of particles through the phase-space boundary at $|\mathbf{u}| = \infty$ (or alternatively from the assumptions about g stated at the end of §2) we have that the integral of $a^i g - \partial(B^{ij}g)/\partial v^j$ over the surface at $|\mathbf{u}| = \infty$ is zero. Using (9a), this becomes

$$\int \left(\beta^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g}{f} \right) - \frac{\phi^i g}{f} \right) dS^i = 0,$$

where dS is an element of the surface at $|\mathbf{v}| = \infty$. Also, on physical grounds, we require that g/f remains bounded as $|\mathbf{v}| \rightarrow \infty$.

The reasoning that follows is similar to that used by Schuss (1980, p. 134). Let us pose an asymptotic expansion for f and ϕ , namely

$$g = g_0 + \epsilon g_1 + \epsilon^2 g_2 + \dots, \quad \phi = \phi_0 + \epsilon \phi_1 + \epsilon^2 \phi_2 + \dots$$

The leading-order (ϵ^{-2}) terms in (21) yield

$$\frac{\partial}{\partial v^i} \left(\beta^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g_0}{f} \right) \right) - \frac{\partial}{\partial v^i} \left(\frac{\phi_0^i g_0}{f} \right) = 0,$$

with g_0/f bounded, and

$$\int \left(\beta^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g_0}{f} \right) - \frac{\phi_0^i g_0}{f} \right) dS^i = 0.$$

Because $\partial \phi_0^i / \partial v^i = 0$, this has a solution $g_0 = C(\mathbf{x}, t)f$; indeed all solutions are of this form. The order- ϵ^{-1} terms in (21) yield

$$\frac{\partial}{\partial v^i} \left(\beta^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g_1}{f} \right) \right) - \frac{\partial}{\partial v^i} \left(\frac{\phi_0^i g_1}{f} \right) = v^i f \frac{\partial C}{\partial x^i}, \quad (22a)$$

with g_1/f bounded, and

$$\int \left(B^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g_1}{f} \right) - \frac{\phi_0^i g_1}{f} \right) dS^i = 0. \tag{22b}$$

The solvability condition for g_1 is $\int v^i f (\partial C / \partial x^i) d^3v = 0$, which is automatically satisfied. The order- ϵ^0 equation becomes

$$\frac{\partial}{\partial v^i} \left(B^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g_2}{f} \right) \right) - \frac{\partial}{\partial v^i} \left(\frac{\phi_0^i g_2}{f} \right) = f \left(\frac{\partial C}{\partial t} + U^i \frac{\partial C}{\partial x^i} \right) + v^i \frac{\partial g_1}{\partial x^i} + \frac{\partial}{\partial v^i} \left(\frac{\phi_1^i g_1}{f} \right),$$

with g_2/f bounded, and

$$\int \left(B^{ij} f \frac{\partial}{\partial v^j} \left(\frac{g_2}{f} \right) - \frac{\phi_0^i g_2}{f} \right) dS^i = 0.$$

The solvability condition for g_2 is

$$\left(\frac{\partial C}{\partial t} + U^i \frac{\partial C}{\partial x^i} \right) \int f d^3v + \frac{\partial}{\partial x^i} \int v^i g_1 d^3v = 0,$$

where g_1 is a solution of (22). Hence, by noting that

$$\int f d^3v = \langle \rho \rangle, \quad \partial \langle \rho \rangle / \partial t + \partial (\langle \rho \rangle U^i) / \partial x^i = 0$$

and $C \propto \langle c \rangle / \langle \rho \rangle$ to leading order in ϵ ,

$$\frac{\partial \langle c \rangle}{\partial t} + \frac{\partial}{\partial x^i} (\langle c \rangle U^i) = \frac{\partial}{\partial x^i} \left(\langle \rho \rangle K^{ij} \frac{\partial}{\partial x^j} \left(\frac{\langle c \rangle}{\langle \rho \rangle} \right) \right),$$

where $K^{ij} = -\int (u^i - U^i) G^j d^3u / (\int g_a d^3u)$, and G^k is a solution of

$$\frac{\partial}{\partial u^i} \left(B^{ij} g_a \frac{\partial}{\partial u^j} \left(\frac{G^k}{g_a} \right) \right) - \frac{\partial}{\partial u^i} \left(\frac{\phi_0^i G^k}{g_a} \right) = (u^k - U^k) g_a,$$

with G^k/g_a bounded, and

$$\int \left(B^{ij} g_a \frac{\partial}{\partial u^j} \left(\frac{G^k}{g_a} \right) - \frac{\phi_0^i G^k}{g_a} \right) dS^i = 0.$$

Although G is not unique, all solutions differ by g_a times a vector function of x and t which does not affect the value of K . Hence the model reduces to a diffusion-equation model. After some algebra it can be shown that K is positive definite and, if $\phi_0 = 0$, symmetric.

Unfortunately it is not always possible to calculate K analytically. However for the class of models in which $(1/g_a)(\partial(B^{ij}g_a)/\partial u^j + \phi_0^i)$ is a linear function of $u - U$, $-L^{ij}(u^j - U^j)$ say (i.e. those models for which a is a linear function of $u - U$ to leading order in ϵ) K can be found and is given by $K^{ij} = (L^{-1})^{ik} V^{kj}$. This class of models includes most models proposed to date. K can also be found easily in one-dimensional models. In such models ϕ_0 is automatically zero and $K = \int (q^2/Bg_a) du / \int g_a du$, where

$$q = \int_{-\infty}^u (u' - U) g_a(x, u', t) du'.$$

In Gaussian turbulence this reduces to

$$K = \int (\sigma^4 g_a / B) du / \int g_a du.$$

We have seen that, if the model satisfies the well-mixed condition, it reduces to

a diffusion-equation model as the Lagrangian timescale tends to zero. The limit $\tau \rightarrow 0$ is, when rescaled, equivalent to $\min(t, \tau_H) \rightarrow \infty$. Hence, in homogeneous stationary turbulence (where $\tau_H = \infty$), the model becomes an eddy-diffusion model as $t \rightarrow \infty$. Also, if the inhomogeneity or non-stationarity is weak (i.e. $\tau_H \gg \tau$) then the model is approximately an eddy-diffusion model for $t \gg \tau$. However, if the inhomogeneity or non-stationarity is stronger (i.e. $\tau_H \lesssim \tau$), then it is not clear whether the model becomes an eddy-diffusion model at large times or indeed whether it should.

If (4) reduces to a diffusion-equation model as the timescale tends to zero, then the model need not satisfy the well-mixed condition. Durbin (1984) suggested that, as well as reducing to a diffusion-equation model as $\tau \rightarrow 0$, a random-walk model should give the correct variance for the particle velocities in homogeneous stationary turbulence. However this is insufficient to ensure that the well-mixed condition is satisfied and, strictly speaking, implies nothing about the behaviour of the model in more general conditions. Hence we see that requiring the model to reduce to a diffusion equation model as $\tau \rightarrow 0$ is a weaker condition than the well-mixed condition.

3.6. Discussion

It has been shown that four out of the five criteria are equivalent and that the fifth criterion is satisfied if any of the others are. In retrospect the equivalence of so many of the criteria is not so surprising; all four of the equivalent criteria demand that some aspect of the model is consistent with the assumed form of g_a , and so the criteria are all of a similar nature. A natural question to ask is: If the well-mixed condition is satisfied, is the model completely consistent with the assumed form of g_a , in the sense that there exists an ensemble of mass-conserving velocity and density fields for which (i) the phase-space density of all the fluid elements equals g_a , and (ii) the stochastic model is exact? If this is so, then it sheds some light on why the well-mixed condition implies the other criteria (if the model is completely consistent with g_a then any criteria involving g_a must automatically be satisfied). In fact the answer is yes. Simply set $\rho(\mathbf{x}, t) = \delta(\mathbf{x} - \mathbf{y}(t)) \int g_a d^3\mathbf{x} d^3\mathbf{u}$ and $\mathbf{u}_E(\mathbf{x}, t) = \mathbf{v}(t)$, where (\mathbf{y}, \mathbf{v}) is a solution of the model (4) with $(\mathbf{y}(0), \mathbf{v}(0))$ having p.d.f. $g_a(\mathbf{y}, \mathbf{v}, 0) / \int g_a(\mathbf{x}, \mathbf{u}, 0) d^3\mathbf{x} d^3\mathbf{u}$. The ensemble of such fields has the required properties. Although the ensemble is rather unphysical (each realization contains only a single particle!) it is sufficient to explain the equivalence of the criteria.

One would like there to be a more physically sensible ensemble with the right properties. It seems likely such an ensemble exists although it is not clear how to prove it rigorously. There must exist a physically sensible ensemble of velocity and density fields $\mathbf{u}_s(\mathbf{x}), \rho_s(\mathbf{x})$ for which the phase-space density of fluid elements equals $g_a(\mathbf{x}, \mathbf{u}, s)$. For each (\mathbf{u}_s, ρ_s) define an ensemble of velocity and density fields $\mathbf{u}_E(\mathbf{x}, t), \rho(\mathbf{x}, t), t > s$, by setting $\mathbf{u}_E(\mathbf{x}, s) = \mathbf{u}_s(\mathbf{x}), \rho(\mathbf{x}, s) = \rho_s(\mathbf{x})$ and letting the fluid elements move according to the model, the same Wiener process $\xi(t)$ being used for all the fluid elements in any particular member of the ensemble. The ensemble formed by superimposing the ensembles formed from each (\mathbf{u}_s, ρ_s) will have the right properties although it is not clear if such an ensemble can be defined for all $t > s$ (for example there is no guarantee that the velocity fields will not develop singularities).

If g_a is such that ρ could be constant (i.e. $\int g_a d^3\mathbf{u}$ independent of \mathbf{x} , $\partial \int u^i g_a d^3\mathbf{u} / \partial x^i = 0$) then one might hope that there exists an ensemble of constant-density flows for which the model is exact, but it is not clear if this is so.

4. The choice of a and B

It has been shown that all the criteria considered above will be satisfied if the well-mixed condition is satisfied, i.e. if a and B satisfy (9a and b). In one dimension (9b) and (10) determine ϕ uniquely and only B is left to be determined since a can then be found from (9a). In more than one dimension however, ϕ is unique only up to the addition of a component that is solenoidal in u -space and tends to zero rapidly as $|u| \rightarrow \infty$. To determine a and B some additional considerations are required. For the remainder of this paper we assume for simplicity that ρ is constant.

4.1. The small-time behaviour of the particles from a point source

It was seen above that the well-mixed condition ensures that certain aspects of the small-time behaviour of particles from an instantaneous point source are correct. However it does not ensure the correctness of all aspects of the small-time behaviour. As in §3.2, we take the point source to be at (x_s, t_s) . At times $(t - t_s) \ll \tau_\eta$, where τ_η is the Kolmogorov timescale, the Lagrangian structure function

$$D^{ij} = \overline{(u^i(t) - u^i(t_s))(u^j(t) - u^j(t_s))}$$

has the form

$$\left\langle \left(\frac{\partial u_{\mathbf{E}}^i}{\partial t} + \mathbf{u}_{\mathbf{E}} \cdot \nabla u_{\mathbf{E}}^i \right) \left(\frac{\partial u_{\mathbf{E}}^j}{\partial t} + \mathbf{u}_{\mathbf{E}} \cdot \nabla u_{\mathbf{E}}^j \right) \right\rangle (t - t_s)^2 + O((t - t_s)^3).$$

At larger times with the time lag $(t - t_s)$ lying in the inertial subrange, D^{ij} has the form

$$D^{ij} = \delta^{ij} C_0 \epsilon (t - t_s), \tag{23}$$

where ϵ is the ensemble-average rate of dissipation of energy and C_0 is a universal constant which has been estimated experimentally to be 4.0 ± 2.0 (Hanna 1981 – our C_0 is Hanna's $2\pi^2 B$). In the model (4) the assumption that (x, u) is a Markov process means that the model can only describe the particle motions correctly on timescales larger than τ_η . Hence we should expect the model to have the form (23) at small times. Now at small times (4) implies

$$D^{ij} = 2\langle B^{ij} \rangle (t - t_s) + O((t - t_s)^2),$$

where $\langle B \rangle$ denotes $\langle B(x_s, u_s, t_s) \rangle$, i.e. $\int B g_a d^3u / \int g_a d^3u$. Hence for accurate results at small times we should choose

$$2\langle B^{ij} \rangle = \delta^{ij} C_0 \epsilon. \tag{24}$$

This was originally suggested by van Dop *et al.* (1985) in the context of a model in which a was a linear function of u . Van Dop *et al.* found that it was impossible in general to ensure that the model structure function had the form (23) at small times while also ensuring that the small-time behaviour of the mean and variance of the particle velocities was correct. If the mean and variance are correct, their model yields a structure function that depends on the inhomogeneity or unsteadiness in the turbulence as well as ϵ . By considering the more general model (4) we have avoided this problem.

It is of interest to calculate the values of $\overline{x^i - x_s^i}$ and $\overline{(x^i - x_s^i)(x^j - x_s^j)}$ at small times. If the model satisfies the well-mixed condition we have, by applying Itô's formula,

$$\overline{x^i - x_s^i} = \langle u_{\mathbf{E}}^i \rangle (t - t_s) + \frac{1}{2} \left(\frac{\partial}{\partial t} \langle u_{\mathbf{E}}^i \rangle + \frac{\partial}{\partial x^j} \langle u_{\mathbf{E}}^i u_{\mathbf{E}}^j \rangle \right) (t - t_s)^2 + O((t - t_s)^3) \tag{25}$$

and

$$\begin{aligned} \overline{(x^i - x_s^i)(x^j - x_s^j)} &= \langle u_E^i u_E^j \rangle (t - t_s)^2 \\ &+ \frac{1}{2} \left(\frac{\partial}{\partial t} \langle u_E^i u_E^j \rangle + \frac{\partial}{\partial x^k} \langle u_E^i u_E^j u_E^k \rangle - \frac{2}{3} \langle B^{ij} \rangle \right) (t - t_s)^3 + O((t - t_s)^4). \end{aligned} \quad (26)$$

Apart from the $-\frac{1}{3}\langle B^{ij} \rangle (t - t_s)^3$ term, which is present because small time in the model means that the time lag $(t - t_s)$ lies in the inertial subrange and not that $(t - t_s) \ll \tau_\eta$, this is in agreement with the correct behaviour obtained by a Taylor expansion (Hunt 1985; van Dop *et al.* 1985). If B satisfies (24) then the term $-\frac{1}{3}\langle B^{ij} \rangle (t - t_s)^3$ is the correct adjustment to the Taylor expansion to account for the fact that $(t - t_s)$ lies in the inertial subrange and is not much less than τ_η (Hunt 1985). It is of interest to note that models in which \mathbf{a} is a linear function of \mathbf{u} do not give the correct expression for the second moments of \mathbf{x} (van Dop *et al.* 1985). This is connected with the inability of such models to satisfy (23) and illustrates again the advantages of considering the more general model (4). The higher-order moments of \mathbf{x} are also consistent with the exact results, although they cannot claim to be necessarily correct. This is because the adjustments to the Taylor expansion due to the fact that $(t - t_s)$ is not much less than τ_η cannot be calculated exactly without making further assumptions about the turbulence.

One way to determine the dependence of \mathbf{a} and \mathbf{B} on \mathbf{u} would be to conduct a conditional-release experiment, i.e. an experiment in which tracer is released only if the velocity at the source is equal to a particular value, \mathbf{u}_s say. (In practice such an experiment would probably be conditional on just one component of velocity or the velocity direction, not the vector velocity.) Then we would have

$$\left. \begin{aligned} \overline{u^i - u_s^i} &= a^i(\mathbf{x}_s, \mathbf{u}_s, t) (t - t_s) + O((t - t_s)^2), \\ \overline{(u^i - u_s^i)(u^j - u_s^j)} &= 2B^{ij}(\mathbf{x}_s, \mathbf{u}_s, t_s) (t - t_s) + O((t - t_s)^2), \\ \overline{x^i - x_s^i} &= u_s^i (t - t_s) + \frac{1}{2} a^i(\mathbf{x}_s, \mathbf{u}_s, t_s) (t - t_s)^2 + O((t - t_s)^3), \\ \overline{(x^i - x_s^i)(x^j - x_s^j)} &= \frac{2}{3} B^{ij}(\mathbf{x}_s, \mathbf{u}_s, t_s) (t - t_s)^3 + O((t - t_s)^4). \end{aligned} \right\} \quad (27)$$

If the value of \mathbf{u}_s is varied, the dependence of \mathbf{a} and \mathbf{B} on \mathbf{u} could be estimated experimentally. Hanna (1979) presented some data in which tetroon trajectories were grouped into cases with the same initial velocity, thus providing data similar to those that could be obtained from a conditional release. These data are consistent with \mathbf{B} being independent of \mathbf{u} and \mathbf{a} depending linearly on $\mathbf{u} - \mathbf{U}$. However these forms for \mathbf{a} and \mathbf{B} cannot both be exactly correct in general without violating the well-mixed condition.

Strictly speaking, inertial-subrange theory requires $(u^i(t) - u^i(t_s))(u^j(t) - u^j(t_s))$ to be independent of $\mathbf{u}(t_s)$ for small $(t - t_s)$ (Monin & Yaglom 1975, p. 359) and it follows from (27) that $\mathbf{B}(\mathbf{x}, \mathbf{u}, t)$ should be independent of \mathbf{u} . However inertial-subrange theory is not exact (Monin & Yaglom 1975, pp. 584–585) and this particular aspect of it is likely to be violated if the local instantaneous dissipation rate is correlated with the velocity. For example, in a convective boundary layer it seems likely that the dissipation is larger in the vigorous updraughts than in the downward-moving air.

4.2. Weakly inhomogeneous flows

In flows that are only weakly inhomogeneous or slightly non-stationary (i.e. $\tau_H \gg \tau$) the classical theory of Taylor (1921) and Batchelor (1949) applies for $t - t_s \ll \tau_H$. It

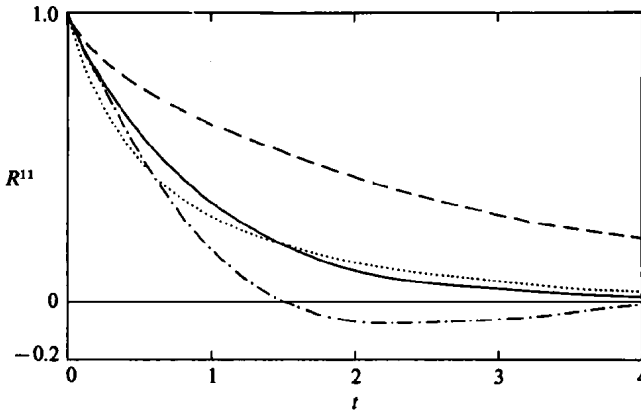


FIGURE 1. Results of numerical calculations of R^{11} in homogeneous stationary Gaussian turbulence with no mean flow and $V^{ij} = \delta^{ij}$ where δ is the Kronecker delta: —, $B^{ij} = \delta^{ij}$, $\phi = 0$; - - -, $B^{ij} = \delta^{ij}$, $\phi = (-u^2, u^1, 0) g_{\mathbf{u}}$; - · - · -, $B^{ij} = (0.2 + (u^1)^2) \delta^{ij} / 1.2$, $\phi = 0$; ····, $B^{ij} = \delta^{ij} / (0.2 + (u^1)^2)$, $\phi = 0$. In the three examples with $\phi = 0$, u^2 and u^3 do not affect u^1 ; hence these are essentially one-dimensional calculations.

follows that, when $t - t_s \ll \tau_H$, the second moments of the spread of the tracer depend only on the Lagrangian correlation function, which is defined by

$$R^{ij}(t) = \overline{u'^i(s) u'^j(s+t)} / (V^{ii} V^{jj})^{\frac{1}{2}}$$

where $\mathbf{u}' = \mathbf{u} - \mathbf{U}$, and on \mathbf{V} (here, and in all other expressions involving \mathbf{R} or τ_i , defined below, the summation convention does not apply). In addition, Pasquill (1974, pp. 131–132) has shown that, if the Lagrangian integral timescales are fixed, the dispersion is relatively insensitive to the shape of \mathbf{R} . It follows that the model should be designed so that the Lagrangian integral timescales $\tau_i^{ij} = \frac{1}{2} \int_0^\infty (R^{ij}(t) + R^{ji}(t)) dt$ are correct. In order to do this it is necessary to be able to calculate the integral timescales of the model. From Batchelor's (1949) theory the timescales of the model are related to the model's diffusivity by $K^{ij} + K^{ji} = 2(V^{ii} V^{jj})^{\frac{1}{2}} \tau_i^{ij}$ and so the timescales can be obtained from the value of \mathbf{K} given in §3.5.

Although the shape of \mathbf{R} does not strongly influence the dispersion, it is of interest to consider what range of shapes can be obtained from a model of the form (4). Unless \mathbf{a} is a linear function of $\mathbf{u} - \mathbf{U}$ it is not clear how to calculate \mathbf{R} analytically, and so some numerical calculations were carried out. The details of the calculation procedure are given in Appendix B and some examples are shown in figure 1 for the case of Gaussian turbulence. The variations in the shape of \mathbf{R} caused by varying \mathbf{B} are small but greater variations can be produced by varying ϕ . The forms of \mathbf{B} and ϕ chosen have no special significance and were chosen simply to provide a range of different shapes for \mathbf{R} .

4.3. Discussion

Changing the form of the dependence of \mathbf{a} and \mathbf{B} on \mathbf{u} has been seen to influence some of the more subtle aspects of the dispersion as predicted by the model, e.g. the dispersion from a conditional release and the shape of the Lagrangian correlogram. However, it is not clear whether all the more subtle aspects can be represented accurately by adjusting \mathbf{a} and \mathbf{B} ; it may well be that, because the true evolution of (\mathbf{x}, \mathbf{u}) is not exactly a Markov process, some aspects can only be represented more

accurately at the expense of the representation of other aspects. In the absence of sufficient data or a theory giving the values of \mathbf{B} and ϕ , it is sensible to keep the model simple. The simplest choice for \mathbf{B} is to choose \mathbf{B} to be independent of \mathbf{u} . This also has the merit of being consistent with inertial-subrange theory. If $\tau_H \gg \tau$, then, in view of Pasquill's result quoted above, \mathbf{B} should be chosen so that the integral timescales of the model are correct. In more general conditions (24) offers what is perhaps the most rational choice for \mathbf{B} . In three-dimensional models a choice also has to be made as to the value of ϕ . It is not clear in general what the simplest choice for ϕ is. Examples are given in the next section.

5. Examples

5.1. Gaussian turbulence

Models of the form (4) which satisfy the well-mixed condition or its equivalent have been used quite extensively in Gaussian turbulence. In homogeneous stationary one-dimensional situations with no mean flow there is the classical Langevin-equation model

$$d\mathbf{u} = -\frac{\mathbf{u}}{\tau} dt + \left(\frac{2\sigma^2}{\tau}\right)^{\frac{1}{2}} d\xi. \quad (28)$$

This satisfies the well-mixed condition and corresponds to (4) with $B = \sigma^2/\tau$ and $a = -\mathbf{u}/\tau$. For this model the Lagrangian correlation function is $\exp(-t/\tau)$ and so τ is the Lagrangian integral timescale τ_L . The first two moments of the Eulerian parametrization are

$$\left\langle c' \left(\frac{D\mathbf{u}_E}{Dt} \right)' \right\rangle = -\frac{\langle c' \mathbf{u}'_E \rangle}{\tau}, \quad (29a)$$

$$\left\langle c' \mathbf{u}'_E \left(\frac{D\mathbf{u}_E}{Dt} \right)' \right\rangle = -\frac{\langle c' \mathbf{u}'_E{}^2 \rangle}{\tau}. \quad (29b)$$

As in §3.3 a prime denotes the departure of a quantity from its ensemble average. These parametrizations are qualitatively sensible and have been used in high-order closure models (Deardorff 1978). Van Dop *et al.* (1985) suggest that (29b) may overestimate the magnitude of $\langle c' \mathbf{u}'_E (D\mathbf{u}_E/Dt)' \rangle$. If a smaller value is deemed desirable, it may be possible to achieve this by allowing B to depend on \mathbf{u} . However this would also alter the parametrization qualitatively.

Generalizations of (28) to more general Gaussian situations have been proposed. These models all make the simplifying assumption that \mathbf{B} is independent of \mathbf{u} . In one dimension ϕ is determined uniquely by the well-mixed condition

$$\frac{\phi}{g_a} = \frac{1}{2} \frac{\partial \sigma^2}{\partial x} + \frac{\partial U}{\partial t} + \frac{1}{2\sigma^2} \left(\frac{\partial \sigma^2}{\partial t} + U \frac{\partial \sigma^2}{\partial x} \right) (u - U) + \frac{1}{2\sigma^2} \frac{\partial \sigma^2}{\partial x} (u - U)^2, \quad (30)$$

and $a = -(B/\sigma^2)(u - U) + \phi/g_a$. As in the Langevin equation it is useful to write

$$B = \frac{\sigma^2}{\tau}. \quad (31)$$

In weakly inhomogeneous or slightly non-stationary conditions (i.e. when $\tau \ll \tau_H$), the arguments in §4.2 show that τ is equal to the Lagrangian integral timescale τ_L . In conditions of stronger inhomogeneity or unsteadiness τ is not the *integral* timescale but simply a (rather loosely defined) 'local decorrelation timescale'. This model is

essentially that described by Wilson *et al.* (1983, equation 3'') and Thomson (1984, §5). The first two moments of the Eulerian parametrization corresponding to (30) and (31) are

$$\begin{aligned} \left\langle c' \left(\frac{Du_E}{Dt} \right) \right\rangle &= k_1 \langle c'u'_E \rangle + k_2 \langle c'u'^2_E \rangle, \\ \left\langle c'u'_E \left(\frac{Du_E}{Dt} \right) \right\rangle &= k_1 \langle c'u'^2_E \rangle + k_2 (\langle c'u'^3_E \rangle - \langle c'u'_E \rangle \sigma^2), \end{aligned}$$

where $k_1 = (1/2\sigma^2)(\partial\sigma^2/\partial t + U\partial\sigma^2/\partial x) - 1/\tau$ and $k_2 = (1/2\sigma^2)\partial\sigma^2/\partial x$. These equations contain terms depending on the inhomogeneity and unsteadiness which are absent in (29). It is hard to assess whether these extra terms yield a more accurate parametrization than (29). To the author's knowledge these terms have not been used to date in high-order closure parametrizations.

In more than one dimension there are many possible choices for ϕ of which the simplest is

$$\begin{aligned} \frac{\phi^i}{g_a} &= \frac{1}{2} \frac{\partial V^{ij}}{\partial x^j} + \frac{\partial U^i}{\partial t} + U^j \frac{\partial U^i}{\partial x^j} + \left(\frac{1}{2} (V^{-1})^{lj} \left(\frac{\partial V^{ll}}{\partial t} + U^m \frac{\partial V^{ll}}{\partial x^m} \right) + \frac{\partial U^i}{\partial x^i} \right) (u^j - U^j) \\ &\quad + \frac{1}{2} (V^{-1})^{lj} \frac{\partial V^{ll}}{\partial x^k} (u^j - U^j) (u^k - U^k). \end{aligned} \quad (32)$$

a is given by $a^i = -B^{ij}(V^{-1})^{jk}(u^k - U^k) + \phi^i/g_a$. The Eulerian parametrization corresponding to this model is similar to the one-dimensional case and is not presented here. The model of Thomson (1986*a*) is slightly different to this formulation with ϕ taking a slightly more complex form. However in the application of the model described by Thomson (1986*a*) the principal axes of V and B were assumed parallel – in these circumstances the model is identical with (32) above. There is no evidence that the more complex form for ϕ is of advantage.

No calculations with these models are presented here; examples can be found in the references cited.

5.2. Skew turbulence

To the author's knowledge, no attempt has been made previously to design a model of the form (4) that can satisfy the well-mixed condition in non-Gaussian turbulence. Here we give a simple one-dimensional example to show that it is possible. The example chosen is the problem of vertical diffusion in free-convective conditions and so z and w will be used as our one-dimensional coordinates.

g_a will be assumed to take the form

$$g_a = \frac{\langle \rho \rangle}{(2\pi)^{1/2} \sigma} \left(\frac{1}{2} s^2 v^2 - sv + 1 - \frac{1}{2} s^2 \right) \exp(-\frac{1}{2} v^2), \quad (33)$$

where $v = w/\sigma - s$ and s is a parameter which may depend on z . Equation (33) implies that $\langle w_E \rangle = 0$ and $\langle w^2_E \rangle = \sigma^2$. To ensure that the third-order velocity moment is correct s must be chosen so that $\sigma^3 s^3 = \langle w^3_E \rangle$. Higher-order velocity moments will of course be incorrect in general (if the higher-order moments are of importance to the dispersion it will be necessary to consider more general forms for g_a such as the sum of two Gaussian distributions as considered by Baerentsen & Berkowicz (1984)). Provided $|s| < 1$, g_a is positive everywhere and, if $s = 0$, the turbulence is Gaussian. Equation (33) was chosen because it is easy to manipulate analytically and depends

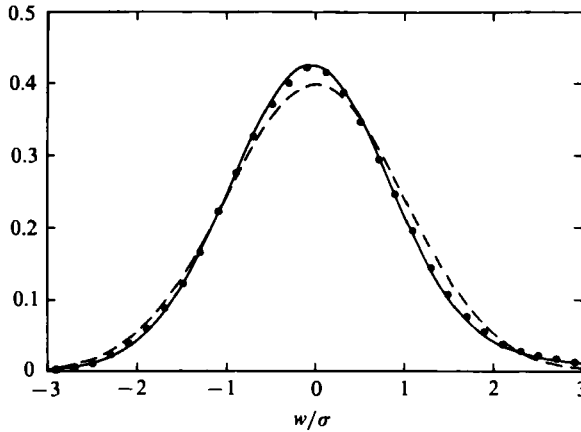


FIGURE 2. Velocity distributions: ----, Gaussian curve; —, equation (33); ●, velocity distribution from the numerical computation, averaged over the time period between 8τ and 10τ after release.

smoothly on w . It is plotted in figure 2 for $s^3 = 0.331$ (the value that will be used in the simulations below). The solution of (9b) for ϕ is

$$\phi = \frac{\langle \rho \rangle}{(2\pi)^{3/2}} \left[\frac{1}{2} v^4 s^2 \frac{\partial \sigma}{\partial z} + v^3 \left((s^3 - s) \frac{\partial \sigma}{\partial z} + \frac{1}{2} s^2 \sigma \frac{\partial s}{\partial z} \right) + v^2 \left(\frac{1}{2} (2 + s^4 - 4s^2) \frac{\partial \sigma}{\partial z} + \frac{1}{2} s^3 \sigma \frac{\partial s}{\partial z} \right) + \frac{1}{2} v (2s - 3s^3) \frac{\partial \sigma}{\partial z} + \frac{1}{2} (2 + s^2 - s^4) \frac{\partial \sigma}{\partial z} - \frac{1}{2} s^3 \sigma \frac{\partial s}{\partial z} \right] \exp(-\frac{1}{2} v^2).$$

B is chosen to be independent of w for simplicity and it follows that a is given by

$$a = -\frac{B}{\sigma} \frac{\frac{1}{2} s^2 v^3 - s v^2 + (1 - \frac{3}{2} s^2) v + s}{\frac{1}{2} s^2 v^2 - s v + 1 - \frac{1}{2} s^2} + \frac{\phi}{g_a}.$$

As in the Gaussian model in §5.1 above, it is convenient to write $B = \sigma^2/\tau$. However, unlike the Gaussian model, τ is not the Lagrangian *integral* timescale even in homogeneous stationary turbulence. To test the model a simulation of homogeneous stationary skew turbulence ($s^3 = 0.331$) was carried out. The initial velocity distribution of the tracer particles was Gaussian. The velocity distribution after a time 8τ is shown in figure 2 and is close to that given by (33).

Consider the free-convective part of a convective surface layer. This is the region where neither u_* (the friction velocity) nor h (the boundary-layer depth) effect the statistical properties of the vertical velocity. In this region, which is found to occupy $|L| < z < 0.1h$, the statistical properties of the vertical velocity depend only on the buoyancy flux $e = u_*^3/|Lk| = w_*^3/h$ where L is the Monin-Obukhov length, w_* is the convective velocity scale and k is von Kármán's constant (Wyngaard, Coté & Izumi 1971; Kaimal *et al.* 1976; Nieuwstadt 1980). The second and third moments of w are given by

$$\langle w^2 \rangle = 1.8(ez)^{2/3}, \quad \langle w^3 \rangle = 0.8ez,$$

where the universal constants 1.8 and 0.8 are taken from van Dop *et al.* (1985). On dimensional grounds τ must take the form

$$\tau = \frac{\alpha z^{2/3}}{e^{1/3}}, \quad (34)$$

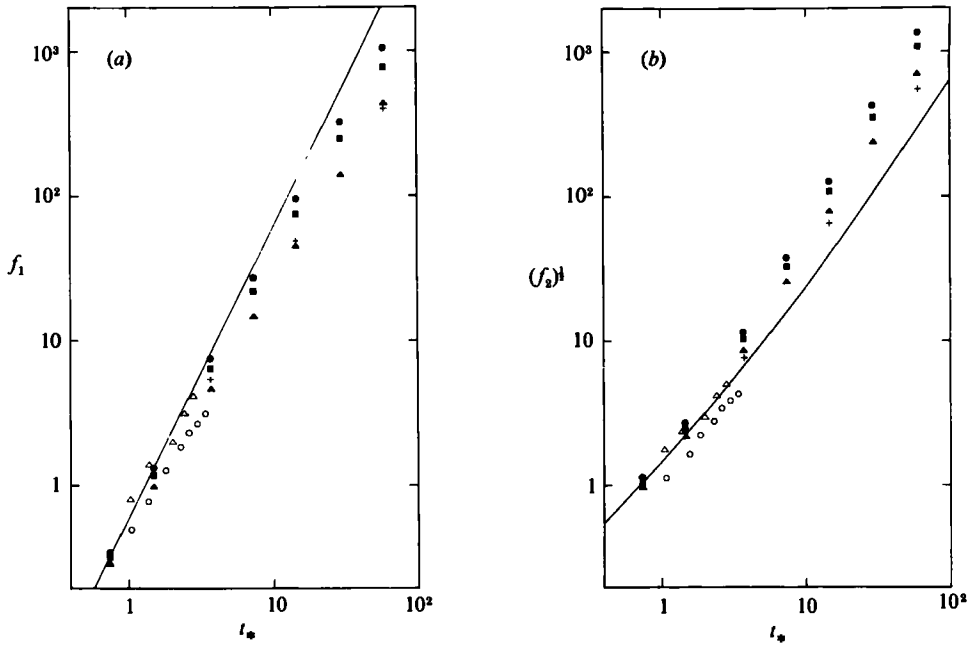


FIGURE 3. Values of (a) f_1 and (b) f_2 from equation (35) and from the random-walk model: —, equation (35), $\alpha = \infty$; ●, random-walk calculation with $\alpha = 2.0$; ■, random-walk calculation with $\alpha = 1.0$; ▲, random-walk calculation with $\alpha = 0.5$; +, random-walk calculation with $\alpha = 1.0$, $\langle w^2 \rangle = 0$; △, Willis & Deardorff's (1976) experimental data, $z_s = 0.05h$; ○, Willis & Deardorff's (1976) experimental data, $z_s = 0.067h$.

where α is a dimensionless constant. If we regard B as being determined by (24), (34) corresponds to ϵ being independent of z which is consistent with similarity theory (Monin & Yaglom 1971, p. 467).

On dimensional grounds the mean and mean-square displacement of particles from an instantaneous point source at $z = z_s, t = 0$ are given by

$$\overline{z - z_s} = z_s f_1(t_*), \quad \overline{(z - z_s)^2} = z_s^2 f_2(t_*),$$

where $t_* = \epsilon t / z_s^2$ and f_1 and f_2 are universal functions. At small times, $t_* \ll 1$, the behaviour of $\overline{z - z_s}$ and $\overline{(z - z_s)^2}$ can be found from (25) and (26):

$$f_1(t_*) = 0.6t_*^2, \tag{35a}$$

$$f_2(t_*) = 1.8t_*^2 + \left(0.4 - \frac{0.6}{\alpha}\right)t_*^3. \tag{35b}$$

It is easy to see that (35a and b) cannot both be correct for t_* much larger than unity without violating the constraint $\overline{(z - z_s)^2} \geq (\overline{z - z_s})^2$. This has consequences for ground-level sources — if $z_s = 0$, t_* is infinite for all $t > 0$ and so (35) cannot be applied.

Information on f_1 and f_2 for $t_* \gtrsim 1$ can be obtained from the random-walk model. The results of the computations are shown in figure 3 and the details of the calculation procedure are given in Appendix B. For small t_* the results show good agreement with (35). At large t_* , f_1 and f_2 are close to being proportional to t_*^2 , which implies that the mean and mean-square displacements become independent of z_s at large t_*

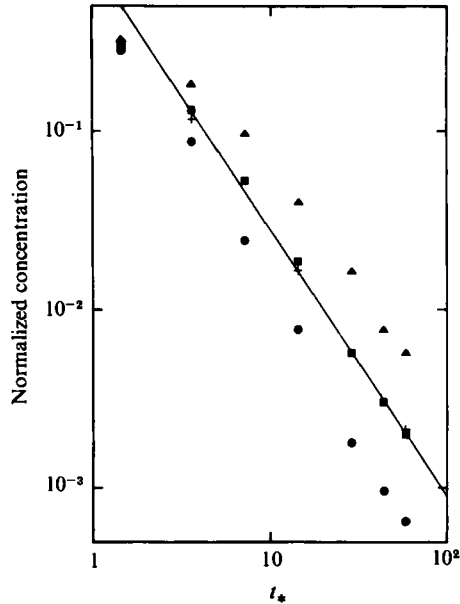


FIGURE 4. Comparison of concentrations from the model (averaged over $0 < z < 2z_s$) with observed ground-level concentrations from a near-surface release: —, observations (Nieuwstadt 1980); ●, random-walk calculation with $\alpha = 2.0$; ■, random-walk calculation with $\alpha = 1.0$; ▲, random-walk calculation with $\alpha = 0.5$; +, random-walk calculation with $\alpha = 1.0$, $\langle w^3 \rangle = 0$.

and that the dispersion from a ground-level source is well behaved. These forms for f_1 and f_2 are consistent with the similarity arguments of Yaglom (1972) for a ground-level source. The results from the random-walk model could be used to estimate the coefficients in Yaglom's formulae for \bar{z} and \bar{z}^2 ; however the values obtained will depend on α . The water-tank data of Willis & Deardorff (1976) are also shown in figure 3. Data for which $\bar{z} > 0.3h$ or $\overline{(z-z_s)^2} > 0.09h^2$ have been excluded since they must be significantly influenced by h . The data are in good agreement with the random-walk and with the small-time result (35) (as was also found by van Dop *et al.* 1985 and Hunt 1985) but do not extend to large enough t_* to enable α to be estimated. A comparison of the ground-level concentrations obtained from the model at large t_* and the observational data analysed by Nieuwstadt (1980) is shown in figure 4. The agreement is best for $\alpha = 1.0$.

Some of the calculations were repeated with $\langle w^3 \rangle = 0$ (see figures 3 and 4). The values of f_1 and f_2 obtained are considerably smaller, showing that the dispersion is quite sensitive to the skewness. The ground-level concentrations are, however, virtually unchanged. It would be of interest to try other forms for g_a to see if the dispersion is sensitive to higher velocity moments or to details in the shape of g_a .

6. Conclusions

We have considered models of particle trajectories in which the trajectories in (\mathbf{x}, \mathbf{u}) -space are Markovian, continuous and have the same local structure as a process with independent increments. Such processes can be represented as solutions of stochastic differential equations of the form (4). This class of models is more general than any considered previously, although it excludes processes with non-Gaussian

forcing; such models are either 'non-existent' (see §2.3) or have discontinuous trajectories.

Various criteria for determining how such models should be formulated in inhomogeneous or non-stationary conditions have been discussed. It has been shown that the well-mixed condition is equivalent to: (i) requiring the small-time behaviour of the velocity distribution of particles from a point source to be correct; (ii) requiring compatibility with the Eulerian equations; and (iii) demanding that the forward and reverse probability densities from the model are consistent. This simplifies the problem of designing a random-walk model because there is no need to consider more than one of these criteria. It has also been found that the well-mixed condition is more restrictive than Durbin's (1984) requirement that the model reduces to a diffusion-equation model as the Lagrangian timescale tends to zero. One of the advantages of considering the general model (4) is that it can be designed to satisfy the above criteria exactly in any situation. The fact that random-walk models can be made consistent with so many of the physical constraints gives increased confidence in such models.

If the well-mixed condition is satisfied then the model is consistent with the known one-point density-weighted Eulerian statistics of the flow. To determine the model uniquely some further assumptions have to be made about the Lagrangian properties of the flow. It has been shown how the model can be designed to have the correct form of the structure function at small times or, if the flow is only weakly inhomogeneous or slightly non-stationary, the correct integral timescales. In contrast to some previous models (van Dop *et al.* 1985) it is always possible, at small times, to ensure that the model's structure function and the second moments of the cloud's spread are consistent with inertial-subrange theory.

To illustrate the theory some examples of models based on (4) and some calculations of dispersion in free-convective conditions have been presented.

The author would like to thank Professor P. C. Chatwin for helpful discussions and suggestions.

Appendix A. Gaussian increments

In §2.3 it was stated that a continuous Markov process with the same local structure as a process with independent increments can be represented by a stochastic differential equation involving a Wiener process. This result follows from the theory presented by Gihman & Skorohod (1974, 1975, 1979) but it is appropriate to give an outline of the proof here in order to explain the most surprising aspect of the result, namely the fact that the infinitesimal increments must be Gaussian.

Before doing this a few comments on the meaning of 'the same local structure as a process with independent increments' are in order. Let us assume (\mathbf{x}, \mathbf{u}) is a Markov process. The increments of (\mathbf{x}, \mathbf{u}) depend on the position and velocity of the particle which in turn depend on the previous increments. Hence (\mathbf{x}, \mathbf{u}) does not form a process with independent increments. However, on physical grounds, the properties of the increments must depend smoothly on \mathbf{x} , \mathbf{u} and t , and so the process behaves like a process with independent increments over short periods of time. To simplify matters let us change notation and consider a continuous Markov process $\mathbf{X}(t)$ in an m -dimensional real vector space R^m (we are interested particularly in the case $m = 6$ with the first three components of \mathbf{X} representing the particle's position and the last three the particle's velocity). Let $p(\mathbf{x}, t | \mathbf{y}, s)$, $\mathbf{x}, \mathbf{y} \in R^m$ be the density corresponding

to the transition probabilities of the process and let $q(x, t | y, s) = p(x + y, t + s | y, s)$ denote the density function of the increment over a time interval $[s, s + t]$. $\hat{q}(\theta, t | y, s) = \int \exp(ix \cdot \theta) q(x, t | y, s) d^m x$ will denote the characteristic function of q . If X were a stochastically continuous process with stationary independent increments we would have \hat{q} independent of y and s , and $\hat{q}(\theta, t_1 + t_2) = \hat{q}(\theta, t_1) \hat{q}(\theta, t_2)$ and so $\hat{q} = \exp(j(\theta)t)$ for some continuous $j(\theta)$. It follows from this that

$$j(\theta) = \lim_{t \rightarrow 0} \frac{\hat{q} - 1}{t},$$

the limit being uniform in each sphere $|\theta| \leq M$ (Gihman & Skorohod 1974, pp. 153–154). Let us define ‘same local structure as a process with independent increments’ to mean that the limit

$$j(\theta, y, s) = \lim_{t \rightarrow 0} \frac{\hat{q} - 1}{t} \tag{A 1}$$

exists uniformly in each sphere $|\theta| \leq M$, is continuous, and also depends ‘smoothly’ on y and s (this will be made more precise below). It seems very unlikely that processes that fail to satisfy this will be physically relevant. In particular the models with non-Gaussian forcing that have been proposed (van Dop *et al.* (1985) and the limit $\Delta t \rightarrow 0$ of the model of Thomson (1984)) satisfy this when they ‘exist’, i.e. when they are realizable. It is well known that limits of the form (A 1) which are continuous in θ and uniform in each sphere $|\theta| \leq M$ can be written in the form

$$j(\theta, y, s) = ia \cdot \theta - B^{ij} \theta^i \theta^j + \int \left(\exp(iz \cdot \theta) - 1 - \frac{iz \cdot \theta}{1 + |z|^2} \right) \frac{1 + |z|^2}{|z|^2} \Pi(d^m z, y, s),$$

where a and B are functions of y and s , and Π is a finite measure given by $\Pi(A, y, s) = \Pi'(A - \{0\}, y, s)$, the measure Π' being the weak limit of the measures

$$\Pi'_t(A, y, s) = \frac{1}{t} \int_A \frac{|z|^2}{1 + |z|^2} q(z, t | y, s) d^m z$$

as $t \rightarrow 0$. For a proof of this result see e.g. Gihman & Skorohod (1974, pp. 154–157).

Let us now assume that the continuous Markov process $X(t)$ has the same local structure as a process with independent increments in the sense defined above. Using an argument similar to that given by Gihman & Skorohod (1974, p. 188) we shall show that, because X is continuous, $\Pi = 0$. Suppose Π is non-zero for $y = y_0, s = s_0$. Then there exist real numbers α_0, γ_0 and δ_0 greater than zero such that

$$\int_{|x| \geq \delta_0} q(x, t | y_0, s_0) d^m x > \alpha_0 t \quad \text{for } 0 < t < \gamma_0.$$

In fact we shall assume that there is a neighbourhood N of (y_0, s_0) and real numbers α, γ and δ (greater than zero) such that

$$\int_{|x| \geq \delta} q(x, t | y, s) d^m x > \alpha t \quad \text{for } 0 < t < \gamma, \quad (y, s) \in N$$

(this follows from the assumption that j depends smoothly on y and s). To simplify notation, choose the origin of time so that $s_0 = 0$ and consider trajectories starting at y_0 at time s_0 . Because the trajectories are continuous there exists $T > 0$

such that $P((X(t), t) \in N, t \in [0, T]) \geq \frac{1}{2}$, where $P(A)$ indicates the probability of event A . Now let $\Delta_h = \sup |X(t_1) - X(t_2)|$, the supremum being taken over all values of t_1 and t_2 for which $|t_1 - t_2| < h$ and $t_1, t_2 \in [0, T]$ and write $t_{nk} = kT/n$ and $\delta X_{nk} = |X(t_{nk}) - X(t_{nk-1})|$. Then

$$\begin{aligned}
 &P(\Delta_{T/n} \geq \delta) \\
 &\geq P(\sup_{k=1 \dots n} \delta X_{nk} \geq \delta) \\
 &\geq P(\delta X_{n1} \geq \delta) + P(\delta X_{n1} < \delta, \delta X_{n2} \geq \delta) + \dots \\
 &\quad + P(\delta X_{nk} < \delta, k = 1 \dots n-1, \delta X_{nn} \geq \delta) \\
 &\geq P(\delta X_{n1} \geq \delta) \\
 &\quad + P(\delta X_{n1} < \delta, (X(t_{n1}), t_{n1}) \in N) P(\delta X_{n2} \geq \delta | \delta X_{n1} < \delta, (X(t_{n1}), t_{n1}) \in N) \\
 &\quad + \dots + P(\delta X_{nk} < \delta, (X(t_{nk}), t_{nk}) \in N, k = 1 \dots n-1) \\
 &\quad \times P(\delta X_{nn} \geq \delta | \delta X_{nk} < \delta, (X(t_{nk}), t_{nk}) \in N, k = 1 \dots n-1) \\
 &\geq P(\Delta_{T/n} < \delta, (X(t_{nk}), t_{nk}) \in N, k = 1 \dots n) \\
 &\quad \times \sum_{l=1}^n P(\delta X_{nl} \geq \delta | \delta X_{nk} < \delta, (X(t_{nk}), t_{nk}) \in N, k = 1 \dots l-1) \\
 &\geq (P(\Delta_{T/n} < \delta) - \frac{1}{2}) \sum_{l=1}^n P(\delta X_{nl} \geq \delta | \delta X_{nk} < \delta, (X(t_{nk}), t_{nk}) \in N, k = 1 \dots l-1).
 \end{aligned}$$

For $n > T/\gamma$ we have

$$P(\Delta_{T/n} \geq \delta) \geq (P(\Delta_{T/n} < \delta) - \frac{1}{2}) \sum_{k=1}^n \frac{\alpha T}{n},$$

and so
$$P(\Delta_{T/n} \geq \delta) \geq \frac{\frac{1}{2}\alpha T}{1 + \alpha T}.$$

In particular $P(\Delta_{T/n} \geq \delta)$ does not tend to zero as $n \rightarrow \infty$, contradicting the continuity of $X(t)$. Hence $\Pi = 0$.

The next step is to derive an equation for the transition probabilities p . Because X is Markovian p obeys the Chapman-Kolmogorov relation

$$p(x, t | y, s) = \int p(x, t | z, r) p(z, r | y, s) d^m z$$

for any r satisfying $s < r < t$. Writing

$$p(x, t | z, r) = \int \tilde{p}(x, t | \theta, r) \exp(i\theta \cdot z) d^m \theta$$

yields
$$\begin{aligned}
 p(x, t | y, s) &= \iint \tilde{p}(x, t | \theta, r) \exp(i\theta \cdot z) p(z, r | y, s) d^m \theta d^m z \\
 &= \int \tilde{p}(x, t | \theta, r) \exp(i\theta \cdot y) \hat{q}(\theta, r-s | y, s) d^m \theta,
 \end{aligned}$$

and so

$$\begin{aligned} \frac{\partial p}{\partial s} &= \lim_{r \rightarrow s} \int \tilde{p}(x, t | \theta, r) \exp(i\theta \cdot y) \frac{1 - \hat{q}(\theta, r-s | y, s)}{r-s} d^m \theta \\ &= \int \tilde{p}(x, t | \theta, r) \exp(i\theta \cdot y) (-i\mathbf{a} \cdot \theta + B^{ij} \theta^i \theta^j) d^m \theta \\ &= -a^i \frac{\partial p}{\partial y^i} - B^{ij} \frac{\partial^2 p}{\partial y^i \partial y^j}. \end{aligned}$$

It follows that the transition probabilities of our process X are identical with those obtained from the stochastic differential equation

$$dX^i = a^i dt + b^{ij} d\xi^j, \tag{A 2}$$

where b is such that $\frac{1}{2}b^{ik}b^{jk} = B^{ij}$, and so our process is stochastically equivalent to that defined by (A 2).

Appendix B. Details of the numerical simulations

The simulations were carried out by replacing the infinitesimal quantities in (4) by finite differences. 20000 particles were followed for the simulations shown in figure 1. For the simulation with B constant and $\phi = 0$ the result can be calculated analytically. A time-step of 0.05 was found to be sufficiently small to achieve good agreement with the analytic result. The same time-step was used for the other case with constant B . For the remaining two simulations in figure 1, $\Delta t = 0.05$ proved unsatisfactory but a time-step of

$$\Delta t = \min\left(\frac{0.05}{B^{11}}, \frac{0.1}{|a|}\right) \tag{B 1}$$

gave results that appeared realistic. (B 1) ensures that a particle cannot change its position in phase space by a large amount in any time-step.

For the simulations in §5, 10000 particles were followed. The time-step $\Delta t = \min(0.05\sigma^2/B, 0.1\sigma/|a|)$, which is just a dimensional version of (B 1), gave good results for the homogeneous simulation (figure 2). In the inhomogeneous case however, a very small time-step, $\Delta t = \min(0.05\sigma^2/B, 0.1\sigma/|a|, 0.01\sigma/|w \partial\sigma/\partial z|)$, was found necessary in order to achieve results that agreed with (35) at small times and that appeared to be insensitive to further reductions in Δt . This value of Δt ensures that the fractional change in σ over a time-step is small. The fact that such a small time-step was required suggests that the use of higher-order finite-difference schemes may be advantageous. The particles were perfectly reflected at the boundary at $z = 0$.

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