MARKOV-CHAIN SIMULATION OF PARTICLE DISPERSION IN INHOMOGENEOUS FLOWS: THE MEAN DRIFT VELOCITY INDUCED BY A GRADIENT IN EULERIAN VELOCITY VARIANCE

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Abstract. The Langevin equation is used to derive the Markov equation for the vertical velocity of a fluid particle moving in turbulent flow. It is shown that if the Eulerian velocity variance σ_{wE} is not constant with height, there is an associated vertical pressure gradient which appears as a force-like term in the Markov equation. The correct form of the Markov equation is:

$$w(t + \Delta t) = aw(t) + b\sigma_{wE}\zeta + (1 - a)T_L\,\partial(\sigma_{wE}^2)/\partial z\,,$$

where $w(t)$ is the vertical velocity at time t, ζ a random number from a Gaussian distribution with zero mean and unit variance, T_L the Lagrangian integral time scale for vertical velocity, $a = \exp(-\Delta t/T_L)$, and $b = (1 - a^2)^{1/2}$. This equation can be used for inhomogeneous turbulence in which the mean wind speed, σ_{wE} and T_L vary with height. A two-dimensional numerical simulation shows that when this equation is used, an initially uniform distribution of tracer remains uniform.

1. Introduction

In many practical situations it is necessary to calculate the mean dispersion of a passive scalar in turbulent flow. Often the diffusion equation gives an adequate solution, for example, for the long-range dispersion of tracers in the atmosphere. However, the diffusion equation is known to fail close to the scalar's source, and also in the complex flow within vegetative canopies (e.g., Wilson and Shaw, 1977, who discuss momentum transport only).

An alternative approach to dispersion is to simulate individual particle trajectories by assuming that the velocity can be represented by a Markov sequence (Thompson, 1971; Hall, 1975; Reid, 1979). Legg (1982), using a single-particle Markov-chain model, compared estimates of vertical dispersion from an elevated line source with results from a wind-tunnel experiment. There was good agreement between model and experiment both close to the source (i.e., at distances less than $\bar{u}T_L$, where $\bar{u}$ is the mean streamline wind speed and T_L is the Lagrangian integral time scale for vertical velocity fluctuations) and distant from the source. Legg also showed that Markov chain models can be generalised to incorporate streamwise velocity fluctuations and skewed velocity distributions. Hence, the Markov chain model shows promise as a replacement for the diffusion equation in predicting the dispersion of passive additives or particles in crop

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canopies, where the turbulent intensity is very high and velocity distributions are skewed.

However, a simple Markov chain model for predicting vertical dispersion is known to fail when the vertical velocity variance changes with height, which always happens within vegetation canopies. Wilson *et al.* (1981a) showed that the simple Markov chain model predicts a large and unrealistic downward drift of particles. Using intuitive, nonrigorous arguments, they suggested several possible ways of removing the drift.

The aim of this paper is to present a rigorous treatment of particle dispersion in a flow with a gradient of velocity variance. To test the theory, we simulate (for vertical fluctuations only) the vertical dispersion of a tracer cloud that is initially uniformly distributed, so that the concentration is constant with height. In a correctly specified dispersion model, such a uniform tracer distribution must remain uniform.

2. The Langevin Equation and Markov-Chain Models of Turbulent Dispersion

Markov-chain simulations of fluid-particle trajectories (Thompson, 1971; Hall, 1975; Reid, 1979; Legg, 1982), in which the particle velocities are represented by a Markov sequence, are based on an assumed equation of motion for a fluid particle. The equation used implicitly in existing models of this kind is the Langevin equation, which describes the motion of a particle subject to a retarding force and a random acceleration: for example, a pollen grain undergoing Brownian motion in a liquid. In fact, this equation was first studied in connection with Brownian motion (e.g., Wang and Uhlenbeck, 1945; Csanady, 1973, p. 28), and was only later applied to turbulent dispersion (e.g., Durbin, 1980). This section shows how the Langevin equation relates to existing Markov-chain models of turbulent dispersion.

The Langevin equation is

$$\frac{\mathrm{d}w}{\mathrm{d}t} = -\alpha w + \lambda \xi(t)\,, \tag{1}$$

where $w(t)$ is the vertical component of a fluid particle, α and λ are coefficients to be specified below and $\xi(t)$ is Gaussian white noise (Arnold, 1974, p. 50), which is a stationary stochastic process with a Gaussian probability density function, a mean of zero and a covariance (at two times s and t) of

$$\overline{\xi(s)\xi(t)} = \delta(t-s)\,, \tag{2}$$

δ being the Dirac delta function and the overbar denoting an ensemble average over many realizations of the stochastic process. Another property of $\xi(t)$ is that it is everywhere discontinuous; however, its integral is a continuous (but not differentiable) process.

Although Equation (1) is a stochastic differential equation, its solution is obtainable by formal application of the conventional method for an ordinary first-order linear differential equation (e.g., Arnold, 1974, pp. 128–134). The solution is

$$w(t) = w(0)e^{-\alpha t} + \lambda \int_0^t e^{\alpha(s-t)}\xi(s)\,\mathrm{d}s\,, \tag{3}$$

which defines the velocity $w(t)$ of a Brownian particle as a random process with the random initial value $w(0)$. By taking the ensemble average of Equation (3), it follows that the mean of $w(t)$ is

$$\overline{w}(t) = \overline{w}(0)e^{-\alpha t} \tag{4a}$$

and that the fluctuation about the mean is

$$w'(t) = w'(0)e^{-\alpha t} + \lambda \int_0^t e^{\alpha(s-t)}\xi(s)\,\mathrm{d}s\,, \tag{4b}$$

where primes denote departures from ensemble-average values (so that $w = \overline{w} + w'$). The variance $\overline{w'^2(t)}$ and the covariance function $\overline{w'(0)w'(t)}$ of $w(t)$ can now be found. Since ξ is uncorrelated with w, the variance is just the sum of the variances of the two terms on the right of Equation (4b); hence

$$\overline{w'^2(t)} = \overline{w'^2(0)}e^{-2\alpha t} + \lambda^2 \int_0^t \int_0^t e^{\alpha(s-t)}e^{\alpha(u-t)}\,\overline{\xi(s)\xi(u)}\,\mathrm{d}s\,\mathrm{d}u\,,$$

which can be simplified, using Equation (2), to

$$\overline{w'^2(t)} = \overline{w'^2(0)}e^{-2\alpha t} + \lambda^2 \int_0^t e^{2\alpha(s-t)}\,\mathrm{d}s\,.$$

By evaluating the integral, we obtain, for the variance of $w(t)$,

$$\overline{w'^2(t)} = \overline{w'^2(0)}e^{-2\alpha t} + \frac{\lambda^2}{2\alpha}\,(1 - e^{-2\alpha t})\,. \tag{5}$$

The covariance function follows directly from Equation (4b):

$$\overline{w'(0)w'(t)} = \overline{w'^2(0)}e^{-\alpha t}\,. \tag{6}$$

These expressions for the variance and covariance of $w(t)$ enable the coefficients α and λ in Equation (1) to be expressed in terms of measurable velocity statistics of the particle. If the Lagrangian integral time scale for the particle's velocity T_L is defined as

$$T_L = (\overline{w'^2(0)})^{-1} \int_0^\infty \overline{w'(0)w'(t)}\,\mathrm{d}t\,,$$

then it is apparent from Equation (6) that

$$\alpha = 1/T_L\,. \tag{7}$$

If, further, $w(t)$ is a *stationary* random process, then Equation (4a) shows that $\overline{w}(t) = 0$, and Equation (5) fixes λ as

$$\lambda = \sigma_w \sqrt{2\alpha} = \sigma_w \sqrt{2/T_{\mathrm{L}}}\,, \tag{8}$$

where $\sigma_w^2 = \overline{w'^2(0)} = \overline{w'^2(t)}$ is the Lagrangian velocity variance. Hence, if the Lagrangian velocity statistics σ_w and T_{L} are known, Equation (1) determines the velocities, and therefore the trajectories, of an ensemble of particles with a prescribed distribution of initial velocity $w(0)$.

The ensemble of velocity functions thus determined constitutes a Markov process. Loosely, a Markov process is a stochastic process $w(t)$ whose behaviour at times subsequent to some time t_0 depends only on $w(t_0)$ and not on $w(t)$ at times prior to t_0 (but see Arnold, 1974, or Wang and Uhlenbeck, 1945, for a precise definition). Equation (3) satisfies this criterion. An important property of a Markov process is that it is continuous but not differentiable. Hence, no Markov process can exactly represent particle velocities in a turbulent flow, which must be everywhere differentiable (otherwise, infinite accelerations would occur). Therefore, Equations (1) and (3) cannot describe exactly the velocities of dispersing marked particles in a turbulent flow.

The relevance of Equation (1) to turbulent dispersion emerges only when we consider the particle velocities at discrete times, $t_0, t_1 \ldots t_n$, where $t_{n+1} - t_n = \Delta t$. If we choose

$$\Delta t \gg T_\lambda\,, \tag{9}$$

where T_λ is the time scale over which the particle *acceleration* remains correlated, then the sequence $\{w_n\} = \{w(t_n)\}$ (where w is here the actual vertical velocity of a dispersing particle) will be a Markov sequence, because w_{n+1} will depend only on w_n and not on w_{n-1} or still earlier values. (The distinction between a Markov sequence and a Markov process is that the former is defined only at discrete times, whereas the latter is defined at all times on a continuous interval.) Successive terms in the Markov sequence $\{w_n\}$ are given by

$$w_{n+1} = a w_n + b \sigma_w \zeta_n\,, \tag{10}$$

where ζ_n is a random number from a Gaussian distribution with zero mean and unit variance. The coefficients a and b are selected, as in the continuous case, to give the sequence $\{w_n\}$ the correct variance σ_w^2 and integral time scale T_{L}. This is easily done by comparing Equation (10) with the solution of the continuous equation, taking the integration interval as (t_n, t_{n+1}). This shows that

$$a = e^{-\alpha \Delta t} = e^{-\Delta t/T_{\mathrm{L}}}\,, \tag{11}$$

and (by comparing the variance of Equation (10) with Equation (5), and using Equation (8)) that

$$\sigma_w^2 b^2 = \frac{\lambda^2}{2\alpha}\,(1 - e^{-2\alpha\Delta t}) = \sigma_w^2 (1 - a^2)\,;$$

so that

$$b = (1 - a^2)^{1/2} . \tag{12}$$

Equations (10) to (12) define the one-dimensional model used by Legg (1982) and others.

We expect T_λ to be of the order of the Taylor microscale of the Lagrangian autocorrelation function (Tennekes and Lumley, 1972), which is a measure of the time over which the particle acceleration remains correlated. Hence, the ratio T_λ / T_L is likely to be of the same order as the ratio of the Taylor microscale to the integral scale for the *Eulerian* autocorrelation function for vertical velocity; in the atmospheric surface layer, for example, this ratio is typically 10^{-2} (Bradley *et al.*, 1981). It is therefore possible to choose Δt so that

$$T_\lambda \ll \Delta t \ll T_L ,$$

ensuring that the sequence $\{w_n\}$ describes turbulent dispersion at times much less than T_L after release (but still greater than T_λ).

[In passing, it is worth noting the analogy between a Markov sequence $\{w_n\}$ for velocity, which describes dispersion when $t \gg T_\lambda$, and a Markov sequence of particle *positions*, which describes turbulent dispersion only when $t \gg T_L$. The latter description is equivalent to the diffusion equation (Monin and Yaglom, 1971, p. 606–612) and hence is applicable only when a gradient-diffusion assumption is valid.]

So far, we have assumed that the turbulence is homogeneous, i.e., that both T_L and σ_w are independent of particle position. When T_L varies with position but σ_w is constant (as in an adiabatic surface layer, for example), Equation (10) can be solved numerically for an ensemble of particles using time steps small enough that T_L for any one particle does not vary strongly over a single step. Several workers have shown that this model describes well the dispersion of a tracer in the surface layer (Hall, 1975; Reid, 1979; Legg, 1982; Wilson *et al.*, 1981b). However, Wilson *et al.* (1981a) point out that the model fails when σ_w varies with position. We now show the correct way of incorporating σ_w variation into the model.

3. Effect of a Changing Velocity Variance

In an incompressible turbulent flow, a gradient in velocity variance is always associated with a mean pressure gradient. This is shown by the mean momentum equation, which can be written in tensor notation (Hinze, 1975, p. 22) as

$$\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial}{\partial x_j} \overline{u_i' u_j'} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial \bar{x}_i} + \nu \Delta^2 \bar{u}_i , \tag{13}$$

where u_i is the Eulerian velocity vector, x_i the position vector, ρ the air density, p the pressure and ν the kinematic viscosity. As before, overbars and primes denote ensemble averages and fluctuations therefrom; the summation convention applies for repeated indices. In a stationary, horizontally homogeneous flow over a level surface, the ground being at $x_3 = 0$, the vertical ($\bar{u}_3$) component of Equation (13) is (neglecting viscous stresses in comparison with Reynolds stresses)

$$\frac{\partial \overline{w_E'^2}}{\partial z} = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial z}, \tag{14}$$

where we have reverted to non-tensor notation, z being the vertical position and w_E the Eulerian vertical velocity component (distinguished from the Lagrangian vertical velocity w). Hence, wherever there is a gradient in $\overline{w_E'^2}$ (for example, in a crop), there is also a mean pressure gradient given by Equation (14). [Additional terms in the mean momentum equation for a crop, resulting from the need to consider horizontal averages (Wilson and Shaw, 1977; Raupach and Shaw, 1982) do not enter Equation (14) unless the canopy elements exert a lift force on the flow, i.e., a drag force with a vertical component. We ignore this case.]

When there is a gradient of vertical velocity variance, the equation of motion for a fluid particle must include a mean force due to the action of the mean pressure gradient on the particle. Hence, Equation (1) must be replaced by

$$\frac{\mathrm{d}w}{\mathrm{d}t} = -\alpha w + \lambda\xi(t) + F, \tag{15}$$

where

$$F = -\frac{1}{\rho}\frac{\partial \bar{p}}{\partial z} = \frac{\partial}{\partial z}\overline{w_E'^2}. \tag{16}$$

The solution of Equation (15) is

$$w(t) = w(0)e^{-\alpha t} + \lambda\int_0^t e^{\alpha(s-t)}\xi(s)\,\mathrm{d}s + F\alpha^{-1}(1 - e^{-\alpha t}), \tag{17}$$

which represents a random process with mean

$$\bar{w}(t) = \bar{w}(0)e^{-\alpha t} + F\alpha^{-1}(1 - e^{-\alpha t}) \tag{18}$$

and with the same variance and covariance function (Equations (5) and (6)) as for the earlier solution with $F = 0$. Hence, for stationary $w(t)$, α remains equal to $1/T_L$ and λ to $\sigma_w\sqrt{2/T_L}$ (see Equations (7) and (8)). If $\bar{w}(0) = \bar{w}(t)$, Equation (18) shows that the particles have a mean drift velocity

$$\bar{w}(t) = F\alpha^{-1} = T_L\,\partial\overline{w_E'^2}/\partial z. \tag{19}$$

As before, we construct a Markov sequence

$$w_{n+1} = aw_n + b\sigma_w\xi_n + c \tag{20}$$

from the Markov process (Equation (17)). Comparison of Equations (17) and (20) shows that

$$c = FT_L(1 - e^{-\Delta t/T_L}) \tag{21}$$

with a and b as before (Equations (11) and (12)). Provided that $\Delta t \gg T_\lambda$ and that Δt is small enough that σ_w and T_L do not change significantly for any one particle over a single time step, Equation (20) will accurately reproduce the velocities of particles dispersing in a flow with varying σ_w and T_L.

To assign σ_w we assume (cf. Legg, 1982) that

$$\sigma_w^2 = \overline{w_E'^2}\,. \tag{22}$$

Equation (20) can then be solved numerically.

The result obtained here for the mean drift velocity $\overline{w}(t)$ is identical with that obtained from the diffusion equation in Fokker-Planck form (Monin and Yaglom, 1971, p. 610) which gives

$$\overline{w}(t) = \frac{\partial(\sigma_w^2 T_L)}{\partial z} = T_L\,\frac{\partial \sigma_w^2}{\partial z} + \sigma_w^2\,\frac{\partial T_L}{\partial z}\,. \tag{23}$$

When T_L is constant, this is the same as Equation (19) with the assumption (22). When T_L and σ_w both vary with z, the first and second drift terms in Equation (23) appear in the Markov chain model, Equation (20), through the term c and the terms in a and b, respectively.

4. Simulation Results

The theory has been numerically tested using model A described by Legg (1982), first with Equations (10) to (12) which do not incorporate a σ_w gradient, and then with Equations (20) and (21), which do. The model is two-dimensional (x, z) and steady state (continuous-source); it calculates the velocities, and hence positions, of tracer particles by assuming a streamwise particle velocity which is always equal to an externally specified local mean Eulerian velocity $\overline{u}(z)$, and a vertical particle velocity which is a Markov sequence generated using Equation (10) or (20). The model gives the streamwise particle flux $F_c(z) = \overline{u}(z)\overline{c}(z)$ through any chosen vertical plane downstream of that at which tracer particles are continuously injected. The local mean particle concentration is then calculated as $\overline{c}(z) = F_c(z)/\overline{u}(z)$.

For both tests, an initially uniform concentration profile was created by releasing particles from 24 equally spaced heights in proportion to $\overline{u}(z)$. The resulting $\overline{c}(z)$ profile was normalised to a mean value of unity (as an integral number of particles was released at each height, the initial concentration was not exactly unity at each height; see Figure 2).

If a uniform, self-preserving concentration profile extends throughout an unbounded atmosphere, all tracer particles diffusing upward through any given plane are replaced

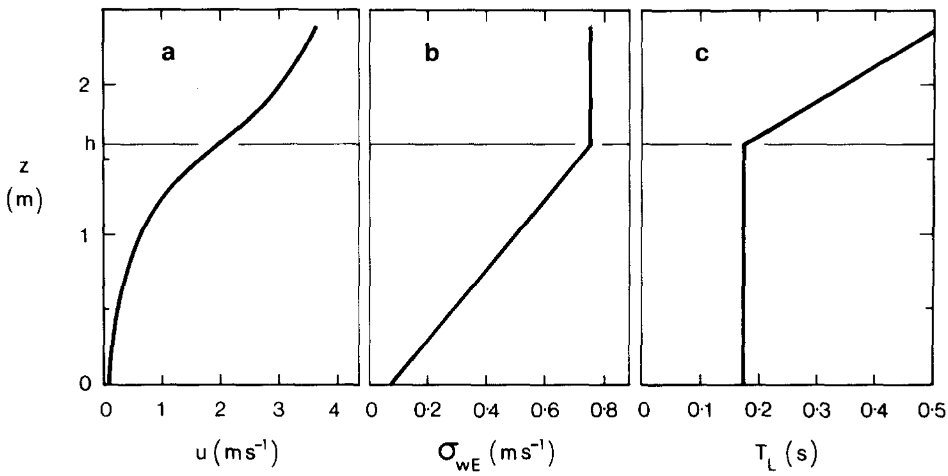

Fig. 1. Profiles of (a) $\bar{u}$, the mean streamwise wind speed; (b) σ_{wE}, the root-mean-square vertical velocity; and (c) T_L, the Lagrangian integral time scale. The height h of the crop is also shown.

by an equal number diffusing downward. Our finite-height simulation modelled this situation by reflecting all particles that reached the upper boundary. Particles were also reflected at the ground, thus imposing a lower boundary condition of zero flux.

Profiles of windspeed, vertical velocity variance, and Lagrangian time scale (Figure 1) were selected to be typical of those found within and above a crop. The wind speed was specified by

$$\bar{u}(z) = \bar{u}(h)\exp\left(\gamma\left(\frac{z}{h} - 1\right)\right) \qquad z \leq h$$

$$\bar{u}(z) = \frac{u_*}{k}\ln\left(\frac{z-d}{z_0}\right) \qquad z > h\,,$$

where γ is the extinction coefficient within the crop, h the crop height, u_* the friction velocity, k (= 0.4) von Karman's constant, d the zero plane displacement, and z_0 the roughness length. The condition that $\bar{u}$ and $\mathrm{d}\bar{u}/\mathrm{d}z$ must be continuous at $z = h$ imposes the restraints that

$$u(h) = (u_*/k)\ln((h-d)/z_0)\,,$$

and

$$u_* = k(h-d)\gamma u(h)/h\,.$$

Values selected were $h = 1.6$ m, $d/h = 0.75$, $\gamma = 3.0$ (Raupach and Thom, 1981) and $\bar{u}(h) = 2.0$ m s^{-1}; it then follows that $u_* = 0.3u(h) = 0.6$ m s^{-1} and $z_0/h = 0.066$.

The vertical velocity variance σ^2_{wE} was chosen so that σ_{wE} was $1.25u_*$ above the crop (Counihan, 1975) and decreased linearly with depth to $0.125u_*$ at $z = 0$ (Wilson, 1980).

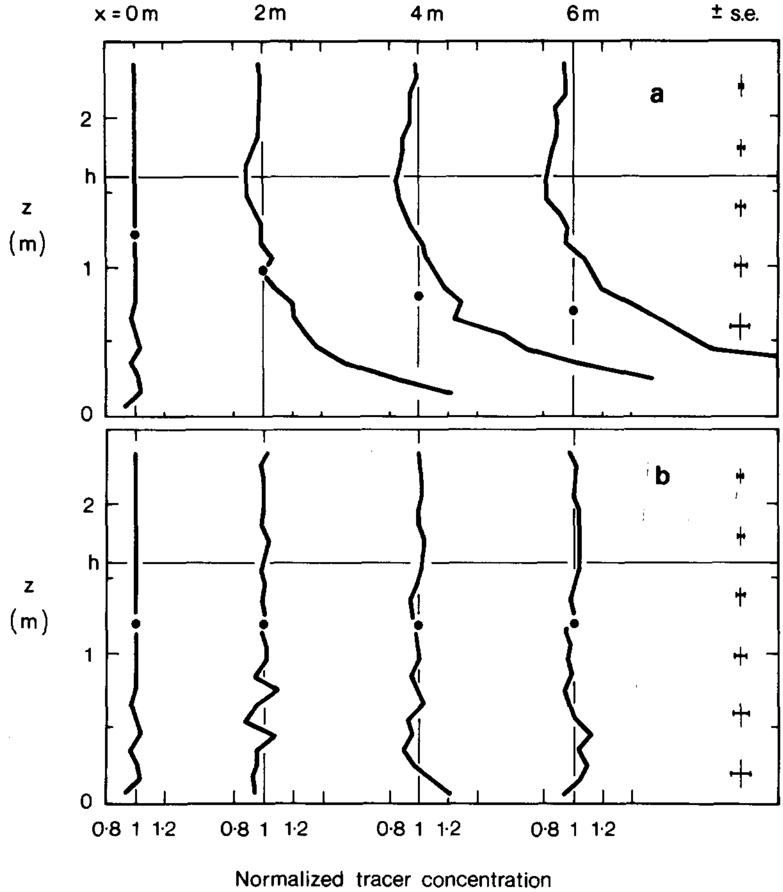

Fig. 2. Normalised profiles of tracer concentration and the height of the concentration centroid (●). Initial concentration profiles ($x = 0.0$ m) were chosen to be approximately uniform. Subsequent profiles were obtained from Markov chain simulations using (a) Equation (10); and (b) Equation (20) with the pressure term included. The symbols (⊢⊣) show ± one standard error and apply to all profiles after $x = 0.0$ m.

The Lagrangian time scale was chosen to increase linearly with $z - d$ above the crop, so that $T_L = 0.32(z - d)/\sigma_{wE}$ (Hunt and Weber, 1979). Within the crop we have assumed, with little evidence, that T_L is constant with height and equals $0.32(h - d)/(1.25u_*)$. For the present simulations, the time step Δt was $0.2\,T_L$. Ten replicates of 4000 particle trajectories gave sufficient accuracy and an estimate of the standard error. The height of the upper boundary was 2.4 m so that the simulation extended 0.8 m above the top of the crop.

The results (Figure 2a) obtained using the Markov model with no pressure force (Equations (10) to (12)) show the downward drift reported by Wilson *et al.* (1981a). After a distance of only 2 m, the concentration close to the ground increased by a factor of 4, and at 6 m by a factor of 10. The downward drift is also shown by the fall of the centroid $\bar{z}$, defined by

$$\bar{z} = \int_0^{z_1} zc(z)\,\mathrm{d}z \bigg/ \int_0^{z_1} c(z)\,\mathrm{d}z\,,$$

where $z_1 = 2.4$ m is the upper limit of the simulation. Initially $\bar{z} = 1.20$ m, but by 6 m it is only 0.71 ± 0.01 m.

Figure 2b shows the results using Equation (20) with the pressure term included. In contrast to Figure 2a, the constant concentration profile is preserved. The scatter in concentration is all within the range expected from the standard errors, the increase in scatter near the ground being caused by the low wind speed and relatively small number of particles contributing to the concentration there. (Of the 40 000 particles used in the simulation, an average of only 128 are below 0.1 m.) The value of $\bar{z}$ is also stable; at 6 m it is 1.196 ± 0.04 m compared with the initial value of 1.20 m.

5. Conclusions

We have shown that the equations commonly used in Markov-chain simulations of particle trajectories in turbulent flow can be derived from the Langevin equation. Furthermore, the pressure gradient associated with a spatial variation of Eulerian vertical velocity variance can be incorporated into the Langevin equation, leading to a modified Markov equation. It also follows from the solution of the Langevin equation that the mean drift velocity induced by a gradient in vertical velocity variance is $\overline{w} = T_L\, \partial \overline{w_E'^2}/\partial z$, the same as that predicted by the Fokker-Planck equation.

A simulation using the modified equation shows that a uniform concentration profile is preserved, as it should be. Thus the equation can be used with confidence in turbulent flows in which mean wind speed, velocity variance, and Lagrangian time scale all vary with height.

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