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A stochastic model for dispersion and concentration distribution in homogeneous turbulence

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A new approach to contaminant diffusion in homogeneous turbulence is proposed. This approach is based on solving for the Lagrangian trajectories of many particles taking into account the interaction among their velocities. The velocity field at a given instant is composed of many 'eddies' distributed randomly and uniformly in space. The velocity of each eddy is proportional to the cube root of its size. In this way the calculated Eulerian correlation function between any two points is consistent with observations. The present model is used to calculate concentration fluctuations, concentration averages and intermittency as functions of location and time. Results were found to be in accordance with experimental measurements. Probability distributions as functions of time and location are also calculated.

1. Introduction

The need for methods of predicting concentration-fluctuation statistics has grown in the last few years. This is because fluctuations about the mean are of the same order of magnitude as the mean itself and therefore cannot be neglected. A method for estimating these fluctuations can be helpful in many fields. For example, in air-quality models, it enables us to predict the frequency with which a given concentration level may be exceeded. Similarly, the probability of visibility through a smoke screen can be predicted. Flammability of a gas cloud and reaction rates depend on concentration covariance. Hazard estimation of toxic gases depends strongly on the short-term concentration levels. In addition, any method that treats contaminants as passive scalars in the turbulent field can also be applied to temperature fluctuations.

There are several models available for calculating the second moment of concentration fluctuations. Some are based on the Eulerian approach, i.e. gradient-transfer approximation or second-order closure to the diffusion equation (see, for example, Csanady 1967; Sykes, Lewellen & Parker 1984). Other models include that based on calculating particle trajectories in a simulated Eulerian field, e.g. Kraichnan (1970); that based on the similarity approach (see Chatwin & Sullivan 1982); and the Lagrangian model using assumptions concerning the Lagrangian velocity statistics (for example, see Durbin 1980; Lee & Stone 1983; Sawford 1985). The main restriction on the gradient-transfer approach is that the lengthscale of the mean field must be larger than that of the turbulence. This restriction is not always satisfied. In the Lagrangian approach assumptions are made about Lagrangian statistics which cannot be measured directly. There are two main approaches to the problem based on different assumptions about the two-particle displacement probability functions. The first approach (Sawford 1985; Lee & Stone 1983) is based on the assumption that the instantaneous rate of separation is a function of the ensemble-mean-square pair separation (Batchelor 1952). The other approach is due to Richardson (Richardson 1926; Durbin 1980), in which the instantaneous rate of separation of a pair of particles is a function of the instantaneous separation of this pair. Durbin's model reproduces the essential features of field and laboratory experiments (see Fackrell & Robins 1982; Hanna 1984). Therefore, it seems that the Lagrangian-statistics assumptions of Durbin's model are more physically meaningful.

In this work, we suggest a new approach to the diffusion problem. The model is based on the calculation of Lagrangian trajectories for N_{P} particles, where N_{P} is large. The trajectory of each particle is obtained by solving a system of Langevin-type equations, but velocities of particles are correlated in space, i.e. the white noise in the equations is spatially correlated. This correlation is assumed to be the same as that between the Eulerian velocities at the particle locations.

The field describing the white noise for velocities is composed of many eddies located randomly and uniformly in space and with random sizes and velocities. A similar description of the structure of a turbulent field is given by Townsend (1976).

N_{R} realizations of trajectories for N_{P} particles are calculated in the present approach, which enables us to estimate the entire distribution of the concentration field and not only the first and second moments. Our model is also capable of predicting other statistical quantities that cannot be predicted by two-particle statistics, like the intermittency – the fraction of non-zero concentration at a given point.

These predictions are compared to the measurement of smoke plumes described by Hanna (1984), and to other two-particle-statistics models.

2. Description of the model

As mentioned above, we suggest a Lagrangian model of the common motion of many particles in the turbulent field. First we assume that the particles move passively in the turbulent field. At $t = 0$ each particle has the velocity of the field at its location, therefore the particle velocities must have the same covariance as the Eulerian field. The second assumption is that the evolution of the velocities of the particles is described by Lagrangian one-particle statistics:

$$V(t+\Delta t) = R_{\mathrm{L}} V(t) + \Theta, \tag{2.1}$$

where R_{L} is the Lagrangian autocorrelation function and Θ is a random velocity field with the same covariance as the Eulerian field. First we shall describe how to construct such a random field, then we shall consider the time evolution.

2.1. *The instantaneous turbulent field*

In this subsection, we describe the construction of a turbulent field which is constrained to fulfil Eulerian correlations in space. This field is based on the description of the turbulent field as a superposition of randomly distributed eddies with random sizes and random energies (see Townsend 1976).

We shall define an 'eddy' of the turbulent motion as a flow pattern with a spatially limited distribution of vorticity. Such an eddy can be defined by its velocity distribution $\boldsymbol{\Theta}_\alpha$ as a function of $\boldsymbol{r}$ relative to its centre:

$$\boldsymbol{\Theta}_\alpha = A_v \boldsymbol{\Phi}(\alpha \boldsymbol{r}), \tag{2.2}$$

where $\Phi(\alpha \boldsymbol{r}) \rightarrow 0$ for $\alpha|\boldsymbol{r}| \rightarrow \infty$. In the present work, we deal with the one-dimensional case and therefore Φ is a function of αZ only, where Z is the one-dimensional coordinate, A_v is the velocity amplitude and $1/\alpha$ is the eddy size. Typical turbulent flows are composed of eddies with a wide range of sizes. The important quantity that we need to describe the turbulent motion is the energy distribution over the range of eddy sizes. This distribution depends on the parameters that characterize the turbulent flow. These parameters are: ϵ, the energy flux that passes from larger to smaller eddies, and ρ, the field density. We assume that the eddy sizes with which we are concerned are much larger than the distance λ_0 at which fluid viscosity begins to be important, and much smaller than L, a characteristic length for the variation of the mean velocity. We shall denote by $V(\alpha)$ the turbulent velocity variation over distance $1/\alpha$. $V(\alpha)$ is determined only by ϵ, ρ, and $1/\alpha$ and the only quantity with dimensions of velocity that can be formed from these three parameters is $(\epsilon/\rho\alpha)^{\frac{1}{3}}$ (see Landau & Lifshitz 1963, p. 121). Therefore, in the range $1/L < \alpha < 1/\lambda_0$ the function that describes an eddy of size $1/\alpha$ centred at the origin is

$$\Theta(Z) = B\left(\frac{\epsilon}{\rho\alpha}\right)^{\frac{1}{3}} \Phi(\alpha Z), \tag{2.3}$$

where B is a dimensionless scalar parameter of order 1. Let us assume that we have a domain which contains eddies of uniform size $1/\alpha$. If the turbulence is homogeneous, in the sense that it contains these eddies with their centres distributed randomly, but statistically uniformly in space, the covariance of the velocity at two different points Z_1, Z_2 is given by

$$\langle \Theta(Z_1)\, \Theta(Z_2) \rangle = \frac{B^2(\epsilon/\rho\alpha)^{\frac{2}{3}}}{A} \int_A \Phi(\alpha(Z_1-\xi))\, \Phi(\alpha(Z_2-\xi))\, \mathrm{d}\xi, \tag{2.4}$$

where the integration is over all turbulent space A. It can be shown that the integral in (2.4) is a function of $\alpha|\Delta Z|$ divided by α, where $\Delta Z = Z_2 - Z_1$ (see Appendix A). Therefore

$$\langle \Theta(Z_1)\, \Theta(Z_2) \rangle = B^2\left(\frac{\epsilon}{\rho\alpha}\right)^{\frac{2}{3}} \frac{1}{\alpha} F(\alpha|\Delta Z|). \tag{2.5}$$

For a turbulent domain that contains eddies of different sizes in the range (λ_0, L), the covariance is given by integrating (2.5) over all α in that range:

$$\begin{aligned}\langle \Theta(Z_1)\, \Theta(Z_2) \rangle &= \frac{B^2(\epsilon/\rho)^{\frac{2}{3}}}{(1/\lambda_0 - 1/L)} \int_{1/L}^{1/\lambda_0} \alpha^{-\frac{5}{3}} F(\alpha|\Delta Z|)\, \mathrm{d}\alpha \\ &= \frac{B^2(\epsilon/\rho)^{\frac{2}{3}} \Delta Z^{\frac{2}{3}}}{(1/l_0 - 1/L)} \int_{|\Delta Z|/L}^{|\Delta Z|/\lambda_0} t^{-\frac{5}{3}} F(t)\, \mathrm{d}t. \end{aligned} \tag{2.6}$$

For $|\Delta Z|/L \gg 1$ the integral in this formula tends to zero and therefore the correlation between two velocities tends to zero. For $|\Delta Z| \rightarrow \lambda_0$, $F(t)$ can be approximated by the first two terms of Taylor's expansion, $C_1 - C_2 t$ where C_1, C_2, are constants independent of α and ΔZ. Therefore, the integral in (2.6) is given by $C_3 - C_4|\Delta Z|^{\frac{2}{3}}$ where C_3, C_4 are constants. From this dependence it can be inferred that the relative velocity between the two points tends to zero like $|\Delta Z|^{\frac{2}{3}}$. The relative velocity dependence on $|\Delta Z|$ is because the main contribution to the velocity difference between two points separated by a distance of $|\Delta Z|$ is from eddies of size $|\Delta Z|$. Eddies of smaller scale will not affect the velocity difference, while eddies of scale much larger than $|\Delta Z|$ contribute very little to the velocity difference. As the

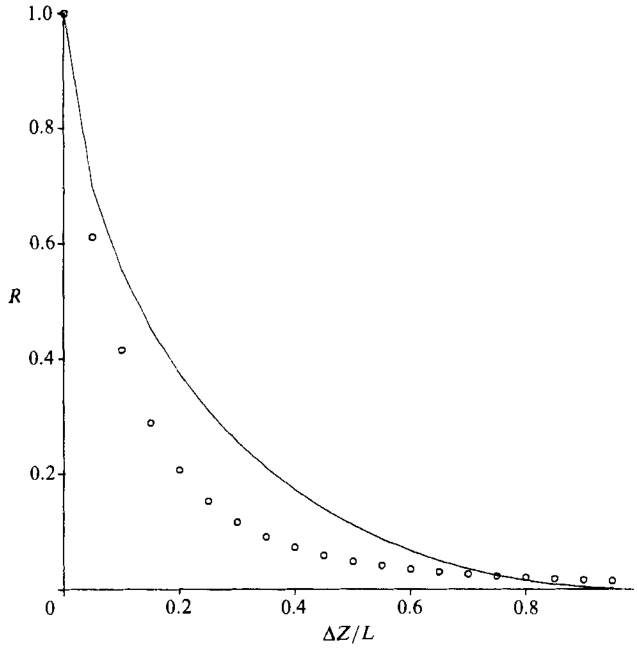


FIGURE 1. Eulerian correlation function R as a function of $\Delta Z/L$. ——, equation (2.8); ○, according to Durbin's (1980) model. The lengthscale of both functions is $0.2L$.

velocity of eddies of size $|\Delta Z|$ behaves like $|\Delta Z|^{\frac{1}{3}}$, the contribution to the velocity difference between two points has the same behaviour.

These consequences do not depend on the specific choice of the function $\Phi(\alpha Z)$ (see (2.2)). For simplicity, we have chosen Φ to be a stepfunction that can be either positive or negative with equal probability:

$$\Phi(\alpha Z) = \begin{cases} \operatorname{sgn}(w-0.5), & |Z| < 1/\alpha, \\ 0, & \text{otherwise,} \end{cases} \tag{2.7}$$

where w is a random variable, uniformly distributed in the interval $(0, 1)$.

In Appendix B, we calculate the correlation function $R(\Delta)$ for $\Phi(\alpha Z)$ defined in (2.7), as well as the variance. The correlation function is given by

$$R(\Delta Z) = \begin{cases} 1-3\,|\Delta Z/L|^{\frac{2}{3}}+2\,|\Delta Z|/L, & |\Delta Z/L| < 1, \\ 0, & \text{otherwise.} \end{cases} \tag{2.8}$$

A graphical representation of R is given in figure 1.

Given this description for the turbulent field, one can construct the velocity field at a given instant as follows. We define a vector in the Z-space. We draw a random number, ξ, from a uniform distribution over range $T, T \gg L$. We draw a random number α from a uniform distribution between $2/L$ and $1/\lambda_0$. These two random numbers describe an eddy centred at ξ with size $1/\alpha$ and velocity proportional to $\alpha^{-\frac{1}{3}}$. Then we add the quantity $\alpha^{-\frac{1}{3}}$ to the velocities of all points Z that are affected by this eddy ($|Z-\xi| < 1/\alpha$). We repeat this procedure N_e times. The velocity at a given point Z is given by

$$\Theta = B\left(\frac{\epsilon}{\rho}\right)^{\frac{1}{3}} \sum_{i=1}^{N_e} \alpha_i^{-\frac{1}{3}}\, \Phi(\alpha(Z-\xi_i)). \tag{2.9}$$

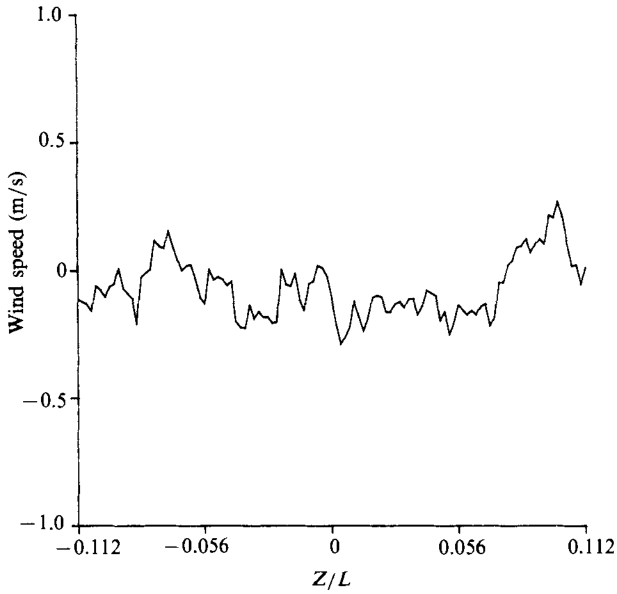


FIGURE 2. A single realization of the fluctuation velocity field at a given time.

The constant B is determined by comparing the calculated variance of the velocity field to a given or measured variance σ_v^2. This yields

$$B = \frac{\sigma_v(T/3N_e)^{\frac{1}{2}}}{(L\epsilon/\rho)^{\frac{1}{3}}} \tag{2.10}$$

(see Appendix B). A single realization of the fluctuation velocity field at a given time is shown in figure 2.

2.2. *Time-Lagrangian autocorrelation function*

We assume that the Lagrangian autocorrelation function for the common motion of the N_P particles is given by an exponential function with integral timescale T_L:

$$R_L(\Delta t) = \exp\left(\frac{-\Delta t}{T_L}\right). \tag{2.11}$$

This function represents the influence on the particle's velocity of the dynamics of the eddies, and the motion of the particles themselves. Changes in flow patterns affecting the correlation can arise either by displacement of any individual eddy, or by a change in the patterns themselves. Three mechanisms can affect the correlation:

(*a*) advection of an eddy centre by the mean velocity field;

(*b*) advection of an eddy centre by the local velocity caused by larger eddies;

(*c*) decay of an eddy amplitude.

Since we use a coordinate system that moves with the mean wind velocity, the first mechanism will not affect the diffusion of the cloud. On the other hand, this mechanism will be dominant in affecting the Eulerian spectra of the velocity field (see § 3). The second mechanism is the dominant one affecting the correlation. The order of magnitude of the timescale of this mechanism is L_E/σ_v, where L_E is the Eulerian lengthscale of the velocity field and σ_v is the standard deviation of the wind velocity at a given point. The contribution of the third mechanism is minor (see Townsend 1967, p. 63). In this work we choose

$$T_{\mathrm{L}} = 0.6\frac{L_{\mathrm{E}}}{\sigma_v}. \tag{2.12}$$

This value has also been used in other works (e.g. Sawford 1983; Durbin 1980).

We assume that the random part of the particles velocities (Θ in 2.1) results from the particles meeting a new set of eddies. Therefore the covariance of the Θ-field is the same as that of the Eulerian field. We would like to emphasize that this is an assumption of the model and, like other assumptions on Lagrangian statistics, cannot be examined directly.

3. Relationship between the Lagrangian timescale and the Eulerian timescale

It is shown in Appendix D, that the Eulerian lengthscale of the velocity field is $L_{\mathrm{E}} = 0.2L$. As $\sigma_v \ll U$, where U is the mean velocity field, the dominant mechanism of destroying the correlation at a fixed point and at a fixed coordinate system is the advection of eddy centres by the mean velocity field. Therefore, the Eulerian timescale T_{E}, typical for the time autocorrelation function at a fixed point, is given by

$$T_{\mathrm{E}} = \frac{L_{\mathrm{E}}}{U} = \frac{0.2L}{U}. \tag{3.1}$$

Using (2.12) and (3.1) one finds the relation between Eulerian and Lagrangian timescales:

$$T_{\mathrm{L}} = \frac{0.6L_{\mathrm{E}}}{\sigma_v} = \frac{0.6UT_{\mathrm{E}}}{\sigma_v}. \tag{3.2}$$

This value is close to the experimental value in Hanna (1981).

4. Motion of particles in the velocity field

Given the Lagrangian correlation function $R_{\mathrm{L}}(\Delta t)$, one can write the equation of motion of a particle. Let us denote by $\Theta(Z)$ a random velocity field that fulfils

$$\langle\Theta^2(Z)\rangle = \sigma_v^2 \quad \text{for any } Z$$

and

$$\langle\Theta(Z_1)\,\Theta(Z_2)\rangle = \sigma_v^2(R(|Z_2-Z_1|) \quad \text{for any } Z_1, Z_2.$$

The construction of $\Theta(Z)$ is described in §2 (see (2.9)). The Lagrangian velocity of a particle in this field is given by

$$V(Z(t+\Delta t)) = R_{\mathrm{L}}(\Delta t)\,V(Z(t)) + [1-R_{\mathrm{L}}^2(\Delta t)]^{\frac{1}{2}}\,\Theta(Z). \tag{4.1}$$

$\Theta(Z)$ is a random field with given spatial correlation and is recomputed at each time step independently of the previous step. It is a sum of many independent random variables, therefore it follows from the central-limit theorem that it is normally distributed with variance σ_v^2. Then the motion of one particle is an Uhlenbeck–

Ornstein process and the probability that the particle is located at point Z after time t, given that its location at time $t = 0$ is Z_0, is (see Wax 1954):

$$P_1(Z) = \frac{\exp\left[-(Z-Z_0)^2/2\sigma_Z^2(t)\right]}{(2\Pi)^{\frac{1}{2}}\sigma_Z(t)}, \tag{4.2}$$

$$\sigma_Z(t) = \surd 2\sigma_V T_L\left(\exp\left(\frac{-t}{T_L}\right)+\frac{t}{T_L}-1\right)^{\frac{1}{2}}. \tag{4.3}$$

With a source described by a distribution of particles $S(Z')$, the average concentration is given by

$$\bar{C}(Z) = \int S(Z')\,P_1(Z-Z')\,\mathrm{d}Z'. \tag{4.4}$$

This formula is consistent with the other Lagrangian-statistics-model estimation of $\bar{C}$ (see Sawford 1983). The innovation in (4.1) is the ability to describe the interaction of N_P particles and their common motion in the turbulent field. This common motion is described by a system of N_P coupled equations defined by

$$\frac{\mathrm{d}Z_i}{\mathrm{d}t} = V(Z_i(t),t), \quad i = 1,\ldots,N_P, \tag{4.5}$$

where $V(Z_i(t),t)$ is given by (4.1).

For example, the equation for the relative velocity of a pair of particles is

$$\begin{aligned} V_r(t+\Delta t) &= V(Z_1(t+\Delta t)) - V(Z_2(t+\Delta t)) \\ &= R_L(\Delta t)\,V_r(t) + (1-R_L^2(\Delta t))^{\frac{1}{2}}\left[\Theta(Z_1(t+\Delta t)) - \Theta(Z_2(t+\Delta t))\right]. \end{aligned} \tag{4.6}$$

As we have shown in Appendix C, $\Theta(Z_1(t+\Delta t)-\Theta(Z_2(t+\Delta t))$ is a random variable normally distributed with variance that depends on the instantaneous separation of the particle pair. The variance σ^2 is given by

$$\sigma^2 = \sigma_v^2\,2[1-R(Z_2(t)-Z_1(t))]. \tag{4.7}$$

In a similar way, the equation for the centre-of-mass velocity of the particle pair is

$$\begin{aligned} V_c(t+\Delta t) &= \tfrac{1}{2}[V(Z_1(t+\Delta t)) + V(Z_2(t+\Delta t))] \\ &= \tfrac{1}{2}\{R_L(\Delta t)\,V_c(t) + (1-R_L^2(\Delta t))^{\frac{1}{2}}\left[\Theta(Z_1(t+\Delta t)) + \Theta(Z_2(t+\Delta t))\right]\}. \end{aligned} \tag{4.8}$$

The sum $\Theta(Z_1(t+\Delta t)) + \Theta(Z_2(t+\Delta t))$ is a random variable with variance $2\sigma_v^2[1+R(Z_1(t+\Delta t)-Z_2(t+\Delta t))]$. We see from this equation that the motion of the centre of mass of the particle pair depends on the instantaneous separation of the particles.

5. The role of molecular diffusion and instrument smoothing

The diffusion process described in §4, poses some puzzles concerning the connection between particle diffusion and contaminant diffusion. It must be emphasized here that by a 'particle' we mean a fluid particle, which is larger than the intermolecular distance but small compared with the variation of velocity scales (much smaller than the smallest eddy dimension λ_0). As the fluid is incompressible, the volume of each fluid particle is constant and in the absence of molecular diffusion, the quantity of contaminant within such a particle is conserved. Therefore, any fluid particle will carry with it the initial concentration of contaminant. The diffusion process described will separate the particles from each other, but will not mix the contaminant that is within them. In such a process, only two discrete values for the concentration are possible at each point; either the initial concentration C_0 or zero. The probability of obtaining the value C_0 will decrease with time, as the particles are displaced one from the other.

This picture is not a physical one and contradicts the experimental evidence.

If we examine the process described in §4, we can see that two particles will move together forever, once the distance between them is smaller than λ_0. This occurs since the particles can be separated only by eddies of the order of magnitude of the distance between them, but the velocity field as defined in §2 includes only eddies greater than λ_0. If the initial source is very small, the chance that two particles coincide is greater and therefore the cloud will not diffuse. In fact, we know that this process does not occur in nature, because at scales of the order of the small-eddy size, molecular diffusion occurs.

In order to solve this problem, we must treat 'particles' not as fluid particles, but as contaminant particles. The velocity of any contaminant particle will be the superposition of the 'fluid-particle' velocity which carries it (see (4.1)) and the molecular diffusion velocity. In our process, we include the molecular diffusion velocity as a random variable derived from a normal distribution with zero mean, and variance σ_m equal to the velocity of the smallest eddies. This formalism prevents two particles from collapsing and moving together permanently, even if they meet. In addition, two particles that are at the same point within the source can arrive at different points after time t. This fact emphasizes the difference between our process – following contaminant trajectories – and Durbin's process (Durbin 1980) – following the 'fluid-particle' trajectory. It also enables us to include the case of small sources of order λ_0 in our formalism.

The smearing of contaminant by molecular diffusion is not rapid in comparison with turbulent diffusion, which separates the particles from each other. Therefore, any particle will carry with it the concentration that is approximately equal to its initial concentration.

Another smoothing process is due to the experimental instruments. Any instrument will average concentration over several fluid particles. The averaging scale of the instrument is large compared to fluid-particle size, but small compared to the turbulence scale. Therefore, in order to calculate concentration at point Z at time t, we sum over all contaminant particles that arrive at a neighbourhood of size V_{λ_0} around Z. This smoothing is similar to that suggested by Durbin (1980), and therefore we adopted his definition of the instantaneous concentration:

$$C = \frac{1}{V_{\lambda_0}} \int_{V_{\lambda_0}} C(Z)\,\mathrm{d}Z, \tag{5.1}$$

where V_{λ_0} is a region of order of the Kolmogorov scale λ_0.

Molecular diffusion is included in our model in order: (i) to prevent particles whose distance is smaller than λ_0 from moving together; and (ii) to include sources of order λ_0. We do not intend that this model should describe fluctuations caused by the dynamic of the fluid in the subinertial range (see for example Sawford & Hunt 1985), and therefore our results are not sensitive to the exact value of σ_m.

6. Numerical methods

6.1. *Particle trajectories*

Particle trajectories are calculated by solving a finite-difference representation of the processes described in §§4 and 5. The set of equations is defined by

$$Z_i(t+\Delta t) = Z_i(t)+\Delta t[V(Z_i(t),t)+V_{\mathrm{m}}(t)], \quad i = 1,\dots,N_{\mathrm{P}}, \tag{6.1}$$

$$V(Z_i(t+\Delta t),t) = R_{\mathrm{L}}(\Delta t)\, V(Z_i(t),t)+[1-R_{\mathrm{L}}^2(\Delta t)]^{\frac{1}{2}}\,\Theta(Z_i(t)) \quad \text{for } i = 1,\dots,N_{\mathrm{P}}, \tag{6.2}$$

where N_{P} represents the number of particles. Since we deal here with an instantaneous source, all the particles are released at time $t = 0$. The initial locations $Z_i(0), i = 1, \dots, N_{\mathrm{P}}$, are determined by the material distribution of the source. For an instantaneous point source located at the origin, we get

$$Z_i(0) = 0, \quad i = 1,\dots,N_{\mathrm{P}}. \tag{6.3}$$

$R_{\mathrm{L}}(\Delta t)$ in (6.2) is defined here by

$$R_{\mathrm{L}}(\Delta t) = \exp\left(\frac{-\Delta t}{T_{\mathrm{L}}}\right) \tag{6.4}$$

(see the discussion in §2.2).

The initial conditions for $V(Z_i(t),t)$ are given by

$$V(Z_i(0),0) = \Theta(Z_i(0)). \tag{6.5}$$

$\Theta(Z_i(t))$ in (6.2) and (6.5) are random velocity fields whose construction is described in §2 (see (2.9)). The parameters involved in the calculation of the random velocity field include: σ_v^2, the variance of the field; λ_0, the smallest eddy size; L, the largest eddy size; N_{e}, the total number of eddies; T_{L}, Lagrangian timescale. Typical values for these parameters are given in §6.4. $V_{\mathrm{m}}(t)$ in (6.1) represents molecular diffusion as described in §5. It is a random variable, normally distributed, with zero mean and variance given by σ_{m}^2.

6.2. *Calculation of the concentration field*

The concentration is estimated by defining a mesh with mesh size ΔZ, and by counting the fraction of particles confined in the interval $(j\Delta Z, j\Delta Z+\Delta Z)$, for $|j| \leqslant M$, and M large enough to contain all the particles. ΔZ should be much smaller than the size of the large eddies but still large enough to contain enough particles that calculation of concentration is meaningful. Typical values are given below.

6.3. *Monte Carlo simulation*

The calculations described in §§6.1 and 6.2 represent a single realization of the process. In order to estimate the statistics described in §7 we need to repeat the process N_{R} times.

6.4. *Typical values of the parameters*

In order to determine the values of the parameters needed in the process, we performed an extensive sensitivity study, particularly for the velocity field, and the final choice of values seems appropriate for our purposes. Typical values are:

$$\begin{aligned}
&\Delta t = 0.05T_L \text{ (s)},\\
&L = 1 \text{ (m)},\\
&T_L = 0.6L_E/\sigma_v = 0.12L/\sigma_v \text{ (s)},\\
&\sigma_v = 0.4 \text{ (m/s)},\\
&\lambda_0 = 1.4\times 10^{-4} \text{ (m)},\\
&N_e \text{ (number of eddies)} = 7000,\\
&N_P \text{ (number of particles)} = 1000,\\
&N_R \text{ (number of realizations)} = 250.
\end{aligned}$$

The number of eddies N_e was chosen by checking the covariance of the random field Θ (see (2.7)). The calculated covariance was compared to the theoretical one (see Appendix B (B 3)) for different values of Z_1 and Z_2. It was found that for $N_e > 5000$ the simulated correlation fitted the theoretical one well.

The number of particles N_P was chosen so that for $t < 2.5T_L$, there would be at least 10 particles in a cell for each realization. N_P selected in this way may result in low accuracy for $t > 2.5T_L$ at the edges of the cloud. The number of realizations N_R was selected so that convergence of the results would be satisfactory.

7. Results

7.1. *The fluctuation statistics*

The diffusion process described in §4.5 is designed for any initial source shape. Analysis was done for a line source that is described by

$$S(Z) = \begin{cases} N & \text{for } |Z| \leqslant l, \\ 0 & \text{for } |Z| > l. \end{cases} \tag{7.1}$$

Three statistical quantities were calculated: the average concentration, the fluctuation intensities and the intermittency – the fraction of non-zero concentration at a point. All these quantities were calculated for selected times as functions of cross-wind distance from the source. Results are shown in figure 3. We see that the average concentration has a Gaussian-shape distribution with standard deviation corresponding to the theoretical estimation:

$$\sigma_Z = \sqrt{2}\sigma_v T_L[\mathrm{e}^{-t/T_L} + t/T_L - 1]^{\frac{1}{2}}. \tag{7.2}$$

In figure 4 the calculated value of σ_Z is compared with the theoretical value. The good agreement shows that the one-particle diffusion process described by (4.1) is equivalent to an Orenstein–Uhlenbeck process.

The fluctuation intensity increases with cross-wind distance from the source. This behaviour is also described by Durbin's (1980) theoretical estimates, and has been found in many experiments (see, for example, Hanna 1984; Ramsdell & Hinds 1971; Fackrell & Robins 1982).

The third statistical quantity that is represented in figure 3 is the intermittency (the fraction of non-zero concentration at a given point). As can be seen, the intermittency decreases with cross-wind distance from the source. This is also in quantitative accordance with experimental results (Hanna 1984; Jones 1983).

In figure 5, the time dependence of the averaged concentration at the source line is shown. This dependence is compared with that of the theoretical formula

$$\bar{C} = 1/[(2\Pi)^{\frac{1}{2}}\sigma_Z(t)]. \tag{7.3}$$

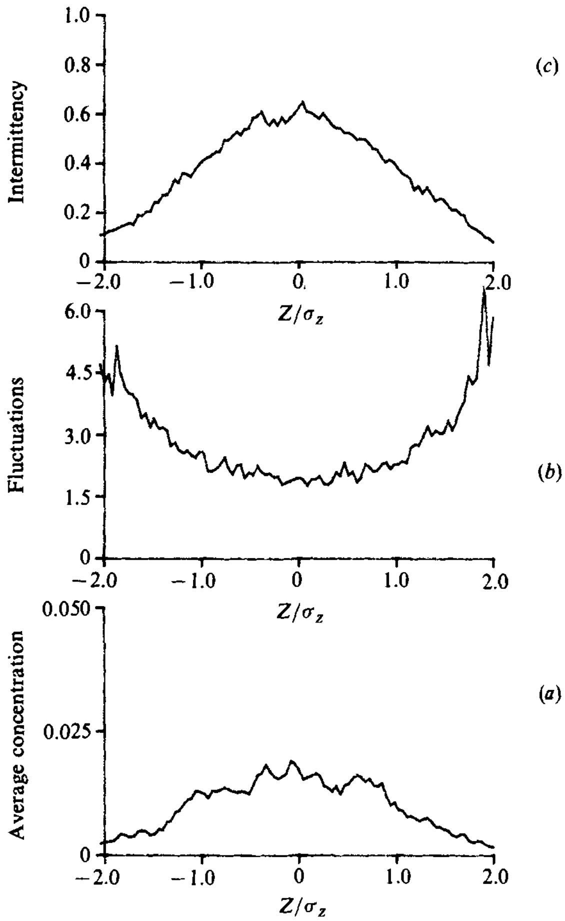


FIGURE 3. Statistical quantities as functions of a cross-wind distance at $t = 3T_L$ for a line source with $l = 4 \times 10^{-4}L$: (*a*) average concentration normalized by total amount of contaminant; (*b*) fluctuation intensity $S = \sigma_C/\bar{C}$; (*c*) intermittency. The cross-wind distance is normalized by σ_z (equation (4.3)).

In figure 6(*a*, *b*) the time dependence of the intermittency and fluctuation intensity on the plume axis, $Z = 0$, are presented. During the first stage, we see that the intermittency decreases with time and then increases. The decrease in time is because, at the beginning, the diffusion is affected by eddies of the same order of magnitude as the cloud size. Since these eddies contain only a small part of the turbulent energy, most of the energy is used for the motion of the cloud as a whole. As a result, most of the time the cloud is absent from the detector and intermittency decreases. Later, when the cloud expands, increasingly larger eddies affect the diffusion process and most of the energy is invested in fluctuations inside the cloud, therefore intermittency of the plume axis increases.

This behaviour of the intermittency also affects the behaviour of the fluctuation intensity as a function of time (see figure 6*b*). At the early stage of the diffusion, intermittency is large because of the presence of the cloud at the detector. At this stage, fluctuations inside the cloud are small and therefore the fluctuation intensity is very small. Later the behaviour of the fluctuation intensity depends on the source

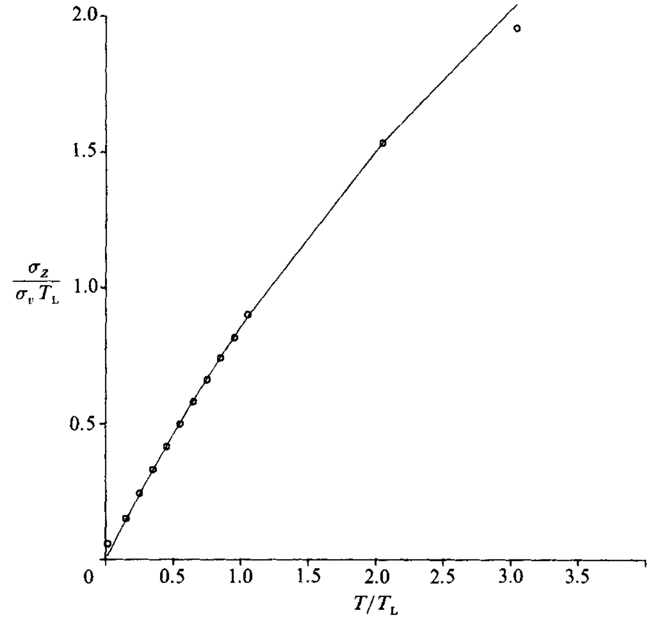


FIGURE 4. The standard deviation of a plume diffused in a homogeneous turbulent field as a function of time for a line source $l = 4\times10^{-4}L$: ——, theoretical value (equation (7.2)); ○, results of our simulation.

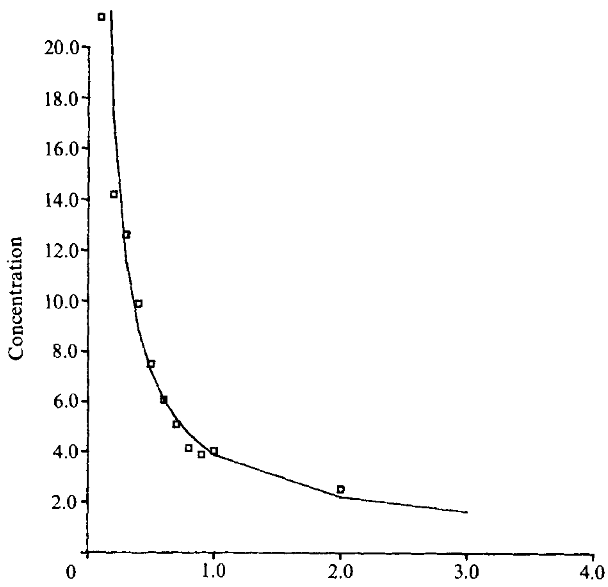


FIGURE 5. Time dependence of averaged concentration normalized by total amount of contaminant, at the source axis, for a line source with $l = 2\times10^{-2}L$: ——, theoretical estimates (equation (7.3)); □, results of the simulations.

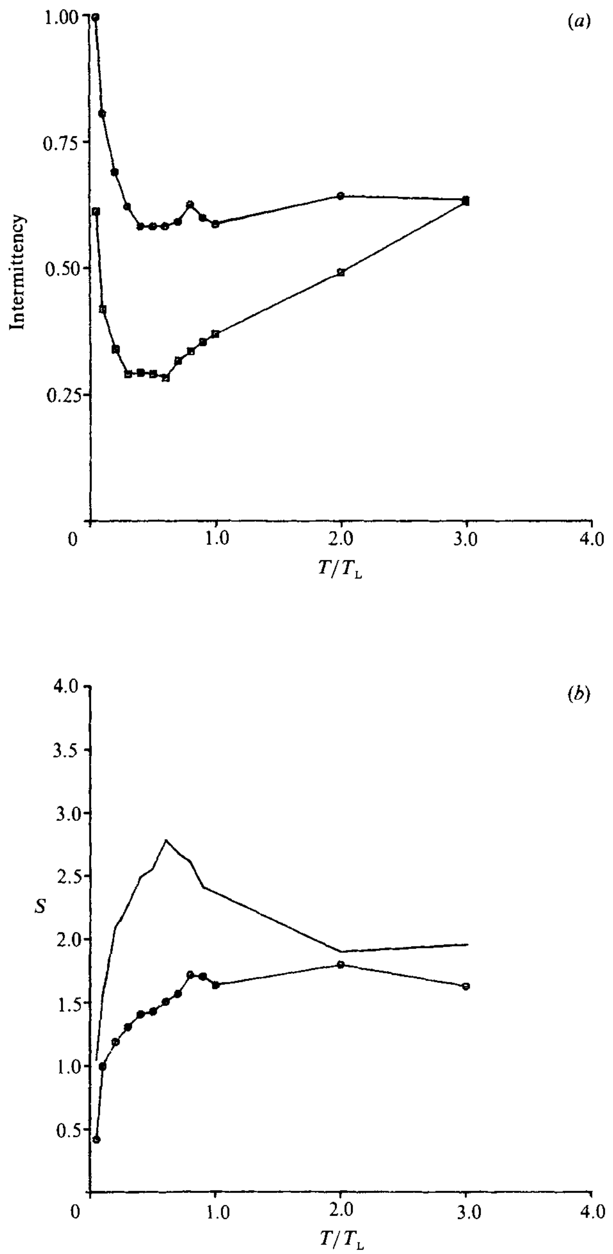


FIGURE 6. (*a*) Time dependence of intermittency at the source axis: □—□, $l = 4 \times 10^{-4}L$; ○—○, $l = 2 \times 10^{-2}L$. (*b*) Time dependence of fluctuation intensity $S = \sigma_C/\bar{C}$ at the source axis: —, $l = 4 \times 10^{-4}L$; ○—○, line source $l = 2 \times 10^{-2}L$.

size. For very small sources, the 'in-plume fluctuations' are substantial but the meandering motion of the cloud is very strong; therefore the fluctuation increases. As the intermittency increases, the fluctuation intensity decreases and tends to its asymptotic value. For larger sources, the time when the meandering motion dominates is very short, and the concentration fluctuation intensity increases to its asymptotic value almost monotonically.

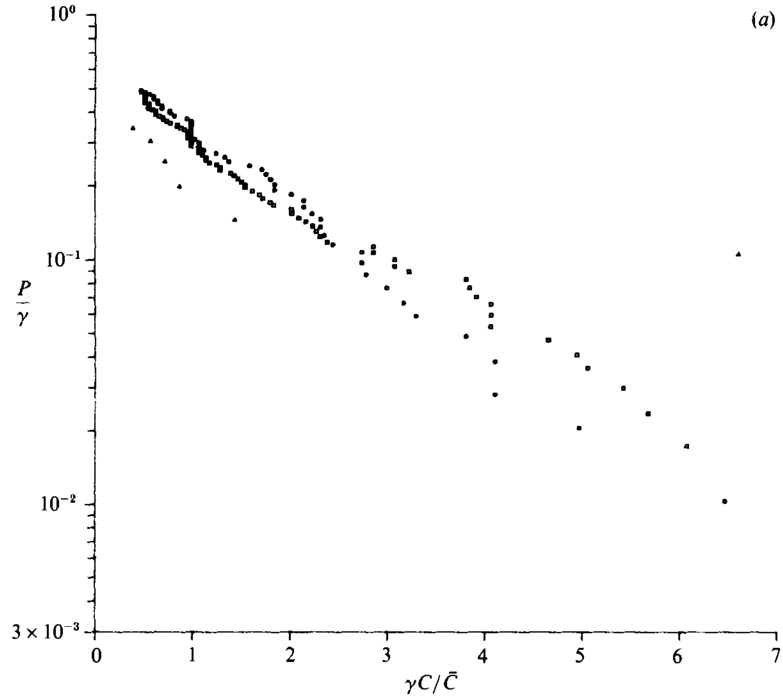


FIGURE 7 (a). For caption see facing page.

7.2. *The concentration distribution function*

For each point and each time the concentration probability distribution function can be calculated. This distribution depends on time, location and initial source size. It is assumed that the non-zero part of the fluctuation distribution can be described by a probability density distribution function $\phi_0(C)$. Then the probability density function $\phi(C)$ depends on the intermittency γ:

$$\phi(C) = \gamma\phi_0(C) + (1-\gamma)\,\delta(C), \tag{7.4}$$

where $\delta(C)$ is the Dirac δ-function. If we denote by $P(C)$ the probability that the concentration at a point exceeds the value C, we get

$$P(C) = \gamma P_0(C), \tag{7.5}$$

where
$$P_0(C) = \int_C^\infty \phi_0(C')\,\mathrm{d}C'.$$

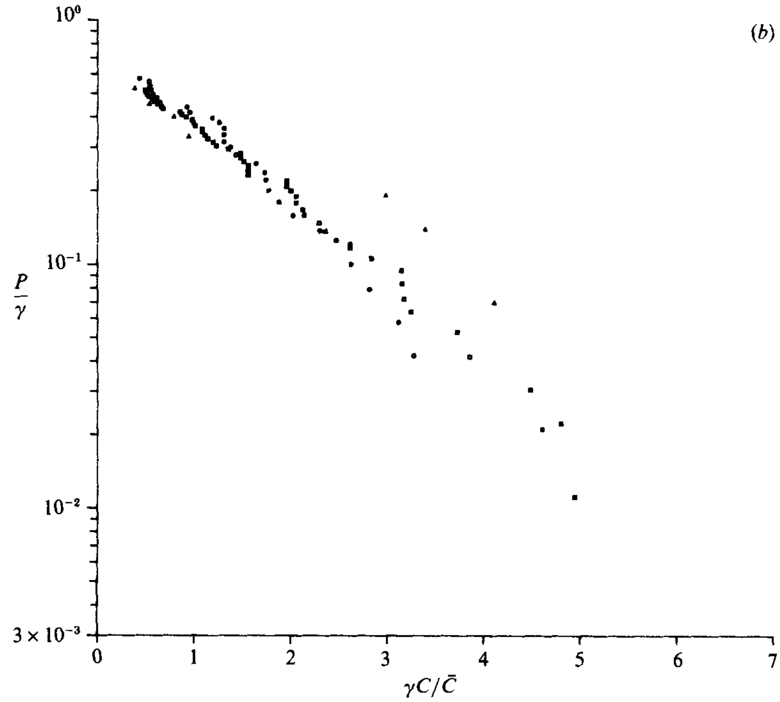
If we assume that the distribution function $\phi_0(C)$ is a function of C/C_0, where

$$C_0 = \int_0^\infty \phi_0(C')\,C'\,\mathrm{d}C', \tag{7.6}$$

we get from (7.4) and (7.6) that $P(C)/\gamma$ is a function of $\gamma C/\bar{C}$.†

Figure 7 is a plot of $P(C)/\gamma$ as a function of $\gamma C/\bar{C}$. This graph shows that this scaling is good for all times. On each plot we draw the distribution at three distances in the cross-wind direction: at $Z = 0$, $0.75\sigma_Z$ and $1.5\sigma_Z$. The three distributions fall approximately on the same curve.

† The above scaling of $\phi_0(C)$ is typical of several distribution functions, like exponential, log-normal, Weibull and others.



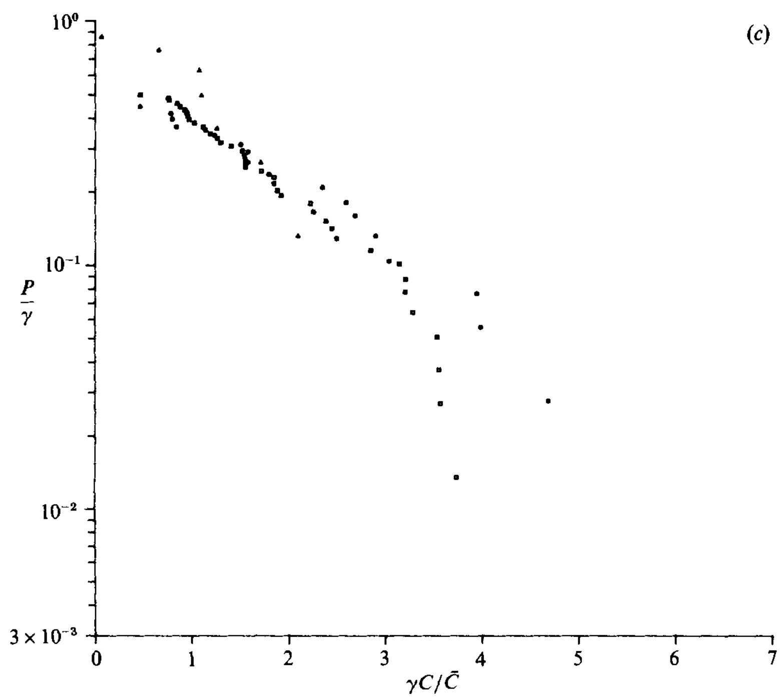


FIGURE 7. The probability of exceeding the concentration value of C normalized by the intermittency γ, as a function of scaled concentration $(\gamma C/\bar{C})$ for the following times t: (a) $3T_L$; (b) T_L; (c) $0.5T_L$ and Z-values: □, 0; ○, $0.75\sigma_z$; △, $1.5\sigma_z$.

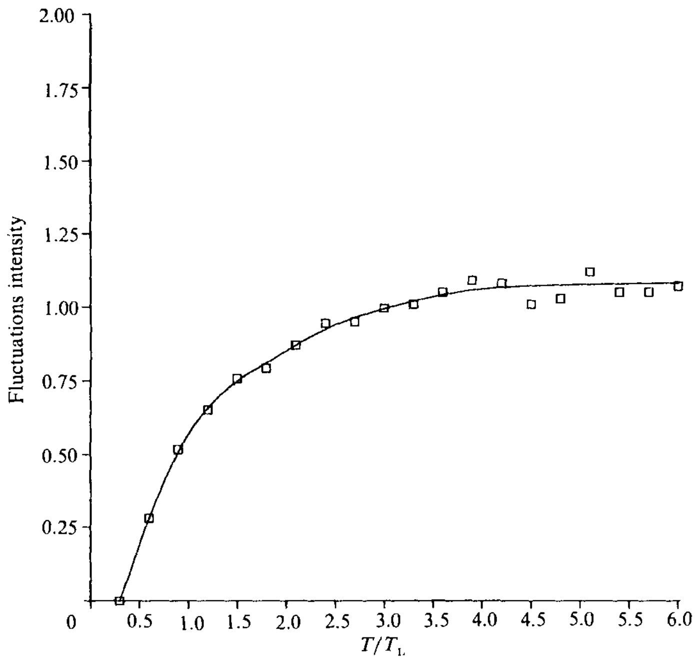


FIGURE 8. Fluctuation intensity as a function of time calculated by the reversed-diffusion process. Source size $l/L_E = 0.1$.

8. Discussion

The model described in this paper is one-dimensional; therefore, like all one-dimensional models (Durbin 1980; Sawford 1985), it describes compressible flow. As was noted by Egbert & Baker (1984), the concentration fluctuations calculated using the forward-diffusion formalism include a contribution from the density fluctuations in the compressible flow; the density fluctuation cannot be isolated and affects the results. Concentration fluctuations can also be calculated using the reversed-diffusion formalism (see Sawford & Hunt 1986; Durbin 1980). The concept of reversed diffusion was introduced by Corrsin (1952) to solve for the initial positions of a pair of particles which are both at point Z at time t. In this formalism, the statistics of C/ρ are calculated (C is the absolute concentration and ρ the fluid density). In order to compare our results to the results of Durbin, we used the concept of reversed diffusion and (4.6) and (4.8) to calculate the fluctuation intensity. Results are described in figure 8. We found that the behaviour of the fluctuation intensity as a function of time is similar to that described by Durbin (1980). It should be emphasized that the fluctuations calculated by the reversed-diffusion process are related to the mass-specific concentration (the ratio between the number of contaminant particles and the number of fluid particles at a given volume) and not the usual definition of contaminant mass per unit volume.

Another point that should be considered is the compatibility of our model with the 'well-mixed' principle analysed by Thomson (1986). This principle claims that if a tracer is well mixed in the flow, then the density function of the distribution in phase space (Z, V) of the tracer particles must be equal to that of the fluid, and therefore unchanged with time. It can be shown that when our model is extended to higher dimensions (Kaplan & Dinar 1986a, b), the model reaches the steady-state solution. On the other hand, the steady-state solution cannot be imposed on a one-dimensional

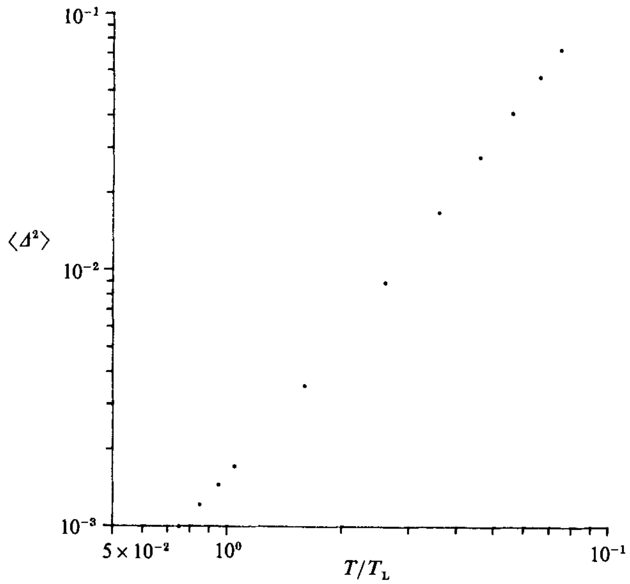


FIGURE 9. The averaged variance of the relative distance of particle pairs as a function of t. The standard dependence $\langle \Delta^2 \rangle = O(t^3)$ is shown.

model (see Kaplan & Dinar 1986*b*). Owing to these two limitations of the one-dimensional model, our approach to the statistics of concentration fluctuation should be extended to higher dimensions. Extension to two-dimensions is given in Kaplan & Dinar (1986*b*).

We also checked our model by calculating the behaviour of $\langle (Z_1-Z_2)^2\rangle$ at small time. Equation (4.6) was solved by numerical simulation. The initial particle separation was zero and the structure function was

$$S(\Delta) = 1-R(\Delta). \tag{8.1}$$

$R(\Delta)$ given in (8.1) was replaced by $R(\Delta_{cr})$ whenever Δ was less than $\Delta_{cr} = 10^{-6}L$ (similar to Thomson 1986). Results presented in figure 9 verify the standard dependence: $\langle (Z_1-Z_2)^2\rangle = O(t^3)$ at small t.

9. Summary

In this work, we describe a new approach to contaminant dispersion in a turbulent medium. The model is based on solving the Lagrangian trajectories of N_P particles, taking into account their interaction. The turbulent velocity field at a given instant is a sum of many 'eddies' which are distributed randomly and uniformally in space. The velocity of each eddy depends on the third root of its size. In such a field, the relative velocity between points is a random variable which depends on the instantaneous separation between them. At a small separation, the relative velocity variance tends to zero as $\Delta^{\frac{2}{3}}$ (where Δ is the relative separation). We have used the definition of concentration proposed by Durbin (1980), which includes smearing effects of molecular diffusion and instrumental averaging. Our model is able to predict the whole distribution of concentration. Intermittency at a fixed point is calculated as well and the results agree quantitatively with experimental behaviour. The concentration probability density function is found to be given by

$\phi(C) = \gamma\phi_0(C\gamma/\bar{C})+(1-\gamma)\,\delta(C)$, where ϕ_0 depends only on source size and not on the point of measurement. Results for the concentration fluctuation intensity are in agreement with Durbin's model and with observed data.

Our model is also able to provide information about the dispersion rate of instantaneous sources, like expansion of the cloud relative to its centre of mass. This will be discussed in a separate paper.

In order to use the model for quantitative predictions that can be compared with observations, the model must be extended to three dimensions and to include the case of inhomogeneous turbulent flow. In principle, extension to three dimensions is straightforward, but computer time may become prohibitive. On the other hand, extension to inhomogeneous turbulence is more difficult and requires further assumptions and approximations.

Appendix A. Velocity correlation for one-sized eddies

The integral on the right-hand side of (2.4) has the form

$$I = \int_A \Phi(\alpha\,|Z_1-\xi|)\,\Phi(\alpha\,|Z_2-\xi|)\,\mathrm{d}\xi. \tag{A 1}$$

It is easy to show that for a class of functions Φ appropriate for describing velocity dependence on the eddy radius, it is true that

$$I = \frac{1}{\alpha\,F(\alpha\,|\Delta Z|)}, \tag{A 2}$$

where $\Delta Z = |Z_2-Z_1|$.

By a change of variables $t = \alpha(Z_1-\xi)$ in (A 1), it can be shown that for $|\Phi(x)|\rightarrow 0$ as $|x|\rightarrow\infty$,

$$I = \frac{1}{\alpha}\int_{A'} \Phi(t)\,\Phi(\alpha\,\Delta Z-t)\,\mathrm{d}t \equiv \frac{F(\alpha\,|\Delta Z|)}{\alpha}. \tag{A 3}$$

Appendix B. The correlation function

The correlation function is given by $\langle\Theta(Z_1)\,\Theta(Z_2)\rangle$ divided by the variance. Let $J = \langle\Theta(Z_1)\,\Theta(Z_2)\rangle$, then

$$J = \frac{1}{T}\int_{2/L}^{\infty}\int_{-T/2}^{T/2} \alpha^{-\frac{2}{3}}H(1-\alpha\,|Z_1-\xi|)\,H(1-\alpha\,|Z_2-\xi|)\,\mathrm{d}\xi\,\mathrm{d}\alpha, \tag{B 1}$$

where
$$H(X) = \begin{cases}1, & x<0,\\ 0, & x\geqslant 0.\end{cases}$$

Using the transformation $\alpha = 1/a$ and results from Appendix A, we obtain

$$J = \frac{2}{T}\int_{\Delta Z/2}^{L/2} a^{-\frac{4}{3}}\int_{Z}^{a+Z_1}\mathrm{d}\xi\,\mathrm{d}a, \tag{B 2}$$

where $\Delta Z = Z_2 - Z_1$ and $Z = \frac{1}{2}(Z_2 + Z_1)$. Therefore

$$\begin{aligned} J &= \frac{2}{T}\int_{\Delta Z/2}^{L/2} a^{-\frac{4}{3}}(a-\Delta Z/2)\,\mathrm{d}a \\ &= \frac{6}{T}\left[\frac{1}{2}\left(\frac{L}{2}\right)^{\frac{2}{3}} - \frac{3}{2}\left(\frac{\Delta Z}{2}\right)^{\frac{2}{3}} - \frac{3}{2}\left(\frac{L}{2}\right)^{-\frac{1}{3}}\left(\frac{\Delta Z}{2}\right)\right] \\ &= \frac{3}{T}\left(\frac{L}{2}\right)^{\frac{2}{3}}(1-3\varDelta^{\frac{2}{3}}+2\varDelta), \end{aligned} \tag{B 3}$$

where $\varDelta = \Delta Z/L$. Dividing by the variance which is obtained from (B 3) taking $Z_2 = Z_1$, i.e. $\varDelta = 0$, we get†

$$R = 1-3\varDelta^{\frac{2}{3}}+2\varDelta \quad \text{for } \varDelta \leqslant 1. \tag{B 4}$$

Appendix C. The relative velocity

The relative velocity of two points Z_1, Z_2 is given by $V_\mathrm{r} = \Theta(Z_1) - \Theta(Z_2)$. Since $\Theta(Z_i)$ is a sum of many independent random variables, equally distributed, it follows by the central-limit theorem that V_r is normally distributed with zero mean and variance given by

$$\begin{aligned} \langle V_\mathrm{r}^2\rangle = \langle \Theta(Z_1) - \Theta(Z_2)^2\rangle &= \langle \Theta(Z_1)^2\rangle + \langle \Theta(Z_2)^2\rangle - 2\langle \Theta(Z_1)\,\Theta(Z_2)\rangle \\ &= 2\sigma_v^2 - 2\sigma_v^2 R(|Z_1 - Z_2|). \end{aligned} \tag{C 1}$$

Appendix D. The Eulerian lengthscale

The Eulerian lengthscale is obtained by calculating

$$L_\mathrm{E} = L\int_0^\infty R(\varDelta)\,\mathrm{d}\varDelta = L\int_0^1 (1-3\varDelta^{\frac{2}{3}}+2\varDelta)\,\mathrm{d}\varDelta = L(1-\tfrac{9}{5}+2\times\tfrac{1}{2}) = 0.2L. \tag{D 1}$$

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† The above calculations hold for $|Z_2 - Z_1| < L$, i.e. $\varDelta \leqslant 1$. It can be seen directly from (A 6) that for $|Z_2 - Z_1| \geqslant L$ the integral vanishes and therefore $R \equiv 0$ for $\varDelta \geqslant 1$.

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