NUMERICAL SIMULATION OF PARTICLE TRAJECTORIES IN INHOMOGENEOUS TURBULENCE, I: SYSTEMS WITH CONSTANT TURBULENT VELOCITY SCALE

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Abstract. A means of numerical simulation of particle trajectories in inhomogeneous turbulence is described. The method employs a simple coordinate transformation which allows a trajectory in inhomogeneous turbulence to be converted to a corresponding trajectory in homogeneous turbulence. Concentration distributions predicted by the trajectory-simulation method agree precisely with analytical solutions in the special cases of homogeneous turbulence, turbulence with power-law wind and eddy diffusivity profiles, and the neutral atmospheric surface layer.

1. Introduction

The Lagrangian approach to turbulent diffusion was introduced by Taylor (1921). However, extension to atmospheric diffusion problems has been difficult because of the inhomogeneity of atmospheric turbulence. As a fluid element moves farther from the ground, it encounters motions of increasing persistence (time-scale) and, in non-neutral stratification, of changing intensity (velocity scale). Because of this difficulty, Eulerian methods prevail in the literature concerning turbulent diffusion, and in the majority of the work the K-theory closure method is employed to relate the turbulent flux to the mean concentration. The weak physical basis for K-theory and consequent limitations on its usage are well known; it is unrealistic to apply K-theory in a system (such as a forest) whose turbulent length scale is large with respect to the distance over which the mean concentration gradient changes significantly (Tennekes and Lumley, 1972; Corrsin, 1974).

In addition to this problem, in order to solve the system of differential equations arising from an Eulerian description, it is usually necessary to employ unrealistic simplifications, for example of the spatial variation of wind speed and eddy diffusivity. Complications such as an elevated source, tracer buoyancy, or non-neutral stratification are very difficult to deal with, and solutions, if obtainable, are quite complex. Numerical solutions, employing realistic higher-order closure methods, are very valuable for some problems, particularly those in which the source strength interacts with the admixture it produces (e.g., evaporation from a reservoir in a desert).

For many problems, a Lagrangian approach is most appropriate. Batchelor

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(1957) introduced the hypothesis of Lagrangian similarity, in a paper concerning diffusion in decaying turbulence in jets and wakes. The hypothesis concerns the relationship between the length, time and velocity scales of the Lagrangian velocity, (Λ_L, τ_L, σ_L) and those of the Eulerian velocity (Λ, τ, σ_w) in inhomogeneous flows. [These scales are precisely defined in Section 2, and the unfamiliar reader is referred to these definitions. Throughout this paper a subscript L implies a Lagrangian property.] Consider a turbulent system in which the Eulerian velocity, w, along the z-axis has root-mean-square value $\sigma_w(z)$ and time-scale $\tau(z)$. Let the Eulerian statistical properties change with z only through $\sigma_w(z)$, $\tau(z)$, $\Lambda = \sigma_w\tau$ ['self-similarity' along the z-axis; for example, if the probability distribution of w is Gaussian at all heights with variance $\sigma_w^2(z)$, the w-distribution is self-similar]. Then if $z(t)$ is the fluid element position and w_L the fluid element velocity along z (whose variance and timescale are $\sigma_L^2(t)$, $\tau_L(t)$) it is hypothesised that

$$\tau_L(t) \propto \tau(z(t))$$

$$\sigma_L(t) \propto \sigma_w(z(t))$$

and that although $w_L(t)$ is a non-stationary function of time, $[w_L(t)]/[\sigma_L(t)]$ is a stationary random function of η, defined by $d\eta = dt/[\tau_L(t)]$.

The hypothesis has been widely employed for atmospheric diffusion problems to deduce restrictions on the form of the concentration profile and behaviour of its moments (see, for example, Cermak, 1962). Examination of experimental data has shown this to be a useful procedure, and has therefore validated the Lagrangian similarity hypothesis.

The Lagrangian similarity hypothesis also provides the basis for a relatively new and very promising alternative approach to turbulent diffusion in inhomogeneous systems, that of numerical simulation of fluid element trajectories. The hypothesis allows one to relate the time-dependent Lagrangian scales to the time-independent Eulerian scales. An ensemble of fluid element trajectories may thereby be constructed, and the concentration distribution resulting from a given source determined.

Numerical simulation of turbulent diffusion by mimicking particle trajectories was first proposed and performed by Thompson (1971), who considered systems in which the Eulerian timescale is independent of position, and formed a record of Lagrangian velocity from a Markov chain. Hall (1974) simulated trajectories in the atmospheric surface layer, assuming that in neutral conditions

$$\tau_L(z) \propto \tau(z) \propto z/\overline{u}(z)$$

where z is height, $u(z)$ is the horizontal velocity, and the overbar denotes a time average. The Lagrangian velocity series was again a Markov chain

$$w_L(t + \Delta t) = w_L(t) \exp(-\Delta t/\tau_L(z)) + [1 - (\exp(-\Delta t/\tau_L(z)))^2]^{1/2}\sigma_w r(t)$$

where r is drawn at random from a Gaussian distribution with variance 1 and mean 0, and σ_w is the standard deviation of the Eulerian vertical velocity. The

timestep Δt was varied with height:

$$\Delta t = \tfrac{1}{8}\tau_L(z).$$

This method is in effect an application of Batchelor's Lagrangian similarity hypothesis. Hall obtained good agreement between predicted and observed cloud heights in the Porton experiments (Pasquill, 1961). It is also demonstrated that if the velocities are chosen completely at random,

$$w_L(t) = \sigma_w r$$

and allowed to persist throughout a large timestep

$$\Delta t = 2\tau_L(z),$$

the resulting spread is not realistic.

Reid (1979) described a simulation method equivalent to that of Hall except that the timescale was chosen

$$\tau_L(z) \propto z/\sigma_w.$$

Use of σ_w rather than $\bar{u}(z)$ is preferable in forming a timescale which relates to dispersion along the vertical axis. Using Reid's choice for the Lagrangian timescale, the eddy diffusivity in the neutral surface layer becomes

$$K = \sigma_w^2 \tau_L \propto z$$

in agreement with the height dependence of the eddy viscosity.

Reid used his simulation model to investigate the accuracy of the Gaussian plume model and of predictions on the form of the concentration profile derived from the Lagrangian similarity hypothesis.

This paper describes a simulation procedure similar to that of Hall and Reid, but with a significant conceptual development which allows particle trajectories in inhomogeneous turbulence to be converted to trajectories in homogeneous turbulence in transformed coordinates. This has practical advantages with respect to the speed and simplicity of the calculation procedure, and provides insight as to the common features of many diffusion problems; all systems with σ_w height-independent become equivalent in the transformed coordinates, except for differences in the shear of the (transformed) horizontal velocity, and the length scale in the transformed system. The simulation method described herein applies to diffusion in two-dimensional flow (wind field (u, 0, w)), but extension to three-dimensional flow is in principle straightforward. The method applies with equal simplicity to diffusion from crosswind line sources and plane sources. This is advantageous for many applications involving diffusion from natural sources, which are often of large areal extent (for example, a barley crop emitting disease spores). Previous methods dealt only with point sources (Thompson) or crosswind line sources (Hall, Reid).

In this paper the trajectory-simulation procedure will be described in detail and its predictions shown to be identical with analytical solutions in special systems. A later paper (II) will consider extension of the method to systems in which σ_w is

height-dependent, and a further paper (III) will present comparisons of predictions of the trajectory-simulation method with experimental data from the atmospheric surface layer. It is hoped that this work will demonstrate the value of the trajectory-simulation method, as a research tool, and as a means of solving practical problems. The method is simple, accurate, and capable of solving a wide variety of problems.

2. A Particle Trajectory in the Neutral Surface Layer

Attention will be confined to calculating trajectories in the neutral surface layer, but the principles are directly applicable to any other situation in which the Eulerian timescale is variable but the Eulerian velocity scale constant. The terms 'particle' and 'fluid element' will be considered equivalent only if the 'particle' is a passive tracer. This is not the case if the particle is heavier than the volume of air it displaces (and in such cases we have given the particle a steady gravitational settling velocity w_g) or if the particle is a molecule of foreign gas which the surface may absorb.

It is assumed that the particle is travelling in a region of the surface layer where the turbulence is stationary and horizontally uniform with the height dependence of the Eulerian scales of the turbulence given by

$$\sigma_w = (\overline{w^2})^{1/2} = a_1 u_*$$

$$\tau(z) = \int_0^\infty R(z, \xi)\, \mathrm{d}\xi = a_2 z/\sigma_w$$

$$\Lambda(z) = \sigma_w \tau(z) = a_2 z$$

where $R(z, \xi)$ is the Eulerian autocorrelation function

$$R(z, \xi) = \overline{w(z, t)\, w(z, t + \xi)}/\sigma_w^2.$$

The position of a particle released at $x = xs$, $z = zs$, $t = 0$ and travelling in a two-dimensional wind field is thereafter given by

$$z = zs + \int_0^t w_L(t)\, \mathrm{d}t$$

$$x = xs + \int_0^t u_L(t)\, \mathrm{d}t.$$

If $w_g \neq 0$, we must add a term $\int_0^t w_g\, \mathrm{d}t$ to z.

In order that simulated trajectories should accurately resemble real ones, it is necessary to decide which of the statistical properties of the fluctuating Lagrangian particle velocity (u_L, w_L) must be reproduced, and which can be regarded as un-

important. Let the instantaneous Eulerian velocities be

$$u = \bar{u} + u'$$

$$w = \bar{w} + w' = w' \qquad (\bar{w} = 0).$$

In the neutral atmospheric surface layer it is found that

$$\bar{u} = (u_*/k) \ln (z/z_0)$$

where u_* is the friction velocity ($u_*^2 = -\overline{u'w'}$), z_0 the roughness length, and k is von Karman's constant. Measurements of $\sigma_u = (\overline{u'^2})^{1/2}$ have usually shown that $\sigma_u \leq 3u_*$ (Haugen, 1973). It follows that when $z \gg z_0$, $\sigma_u \ll \bar{u}$. Furthermore, since $\overline{u'} = 0$, as long as the travel time for a particle moving from $x = 0$ to $x = X$ is large with respect to $\tau_{u'}$, the timescale of u', the effect of u' averages to zero. Now as $z \to 0$, $\tau_{u'} \to 0$. Therefore for long fetch X from source to collector, u' has little effect on the travel time, and consequently little effect on the vertical dispersion (which is of predominant interest for a continuous source in the two-dimensional flow under consideration). Accordingly we have made the approximation $u' = 0$, so that

$$u_L(t) = u(z(t)) = (u_*/k) \ln (z/z_0).$$

The most serious difficulty arising from this approximation is that in the real surface layer, the correlation $\overline{u'w'}$ implies that an upward-moving fluid element systematically has $u' < 0$ ($u < \bar{u}$), and vice versa for downward motion. Our neglect of this systematic behaviour probably leads to some error. However, Hall, who implemented a simple approximation of the correlation between u' and w', states that it is not of major importance.

The fluctuating Lagrangian vertical velocity $w_L(t)$ is not a stationary function of time. As a particle moves farther from the surface, it experiences motions with increasing timescale. Experiments to determine the Lagrangian scales are in concept possible but in practice extremely difficult, and it is therefore necessary to assume relationships between the Lagrangian scales and the (readily measured) Eulerian scales. We could perform an ensemble of experiments in each of which at $t = 0$ we release a particle and measure its velocity w_L at a particular time t, from which we may form an ensemble (E) averaged variance

$$\overline{w_L^2}^{\mathrm{E}}(t, zs).$$

When the Eulerian velocity scale is height-independent, it seems reasonable to assume

$$\overline{w_L^2}^{\mathrm{E}}(t, zs) = \sigma_w^2.$$

This has been proven to be true for the special case of stationary homogeneous turbulence (Tennekes and Lumley, 1972).

The Lagrangian autocorrelation function may be defined by considering an ensemble of releases of individual marked fluid elements at a given height z at time

$t = 0$. Each fluid element is followed after its release, and

$$R_L(z, \xi) = \overline{w_L(t|z)\, w_L(t + \xi|z)}^{E} / \overline{w_L^2}^{E}$$

where $w_L(t|z)$ is the velocity at t of a fluid element which was at z when released. The Lagrangian timescale is defined by

$$\tau_L(z) = \int_0^\infty R_L(z, \xi)\, \mathrm{d}\xi.$$

We assume $\tau_L(z) \propto \tau(z)$. In the neutral surface layer the eddy viscosity is given by

$$K_m = 0.4 u_* z.$$

We therefore expect $\tau_L(z) \propto z$ (because the diffusivity is the product of length scale times velocity scale, and the velocity scale is constant). In (III) the constant of proportionality is determined by comparison of predictions with experimental data.

In summary, we know that as we follow a particle, the persistence of its velocity, which must be considered if the motion is to be simulated, is variable in time. It is not formally possible to translate time-dependence to height-dependence, but we have assumed

$$\frac{\mathrm{d}\tau_L(t)}{\mathrm{d}t} \propto \frac{\partial \tau}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t} = w_L \frac{\partial \tau}{\partial z}.$$

If a particle travels a horizontal distance δX without departing greatly from z, the number of timescales elapsed during the process is

$$[\delta X / u(z)] / \tau_L(z).$$

This ratio of travel time to timescale, which is a measure of the number of independent velocity 'choices', will be preserved if we simulate the particle trajectory by a series of steps in which

$$\begin{aligned} \Delta z &= w_L(t)\, \Delta t = w_L(t_H) \frac{\tau_L(z)}{\tau_L(H)} \Delta t_H \\ \Delta x &= u(z)\, \Delta t = u(z) \frac{\tau_L(z)}{\tau_L(H)} \Delta t_H \end{aligned} \tag{1}$$

where $w_L(t_H)$ is a stationary random function of t_H having r.m.s. value σ_w and timescale $\tau_L(H)$ and t_H is related to real time t by

$$\frac{\mathrm{d}t_H}{\tau_L(H)} = \frac{\mathrm{d}t}{\tau_L(z)}.$$

Steps in t_H time differ from steps in real time except if the particle is at the 'reference height', H. $w_L(t_H)$ must be a record of velocity with time and velocity scales appropriate to particle motion at H (to be discussed later). The choice of reference height

H is completely arbitrary; one may choose any height within the domain in which the turbulence scales are specified (i.e., any height within the domain in which the particles are confined).

It is advantageous to define

$$dz_* = w_L(t_H)\, dt_H$$

and to perform the calculation of trajectories in the transformed coordinate system (x, z_*, t_H) in which the vertical motions have equal timescale at all heights, corresponding to homogeneous turbulence (but with wind shear). This avoids bias resulting from the need to multiply the displacement $w_L(t_H)\Delta t_H$ by a function which changes during the displacement. At any time t_H the real height of the particle may be obtained by integrating

$$dz = \frac{\tau_L(z)}{\tau_L(H)}\, dz_*.$$

For the neutral surface layer, integration gives

$$z = z_2 \exp(z_*/H).$$

Here z_2 is the constant of integration. z_* is logarithmically related to real height. The choice of z_2 is related to the lower boundary condition. First consider a totally reflecting boundary (appropriate for diffusion of marked fluid elements). Reflection occurs at $z = z_2$ ($z_* = 0$) rather than at $z = 0$. Now z_2 can be chosen arbitrarily close to ground, so let us consider $u_2 = u(z_2)$ to be small. Then when a particle travels down to z_2, there is no need to calculate that part of its trajectory below z_2 because we know that when it reappears at z_2 after a real time interval δt, its horizontal position will have changed by $\delta x < u_2 \delta t$, which is small as long as δt is small. If we estimate

$$\delta t \simeq z_2/\sigma_w$$

and are prepared to accept any $\delta x \ll X$ where X is the total horizontal distance travelled, then reflection at z_2 is adequate if

$$\delta x \simeq u_2 z_2/\sigma_w \ll X$$

i.e.

$$u_2 \ll (X/z_2)\sigma_w.$$

Most often we have used $z_2 = z_0$ so that according to the logarithmic wind profile, $u_2 = 0$ and the above constraint is satisfied. Because the logarithmic wind profile is in reality only valid for $z \gg z_0$, this is still a simplification of the process of reflection off the surface, but the above reasoning suggests that the simplification will introduce negligible error into the calculated trajectory $z(x)$.

The case where the lower boundary may absorb particles is more complex. If the particles under consideration have a settling velocity, then total absorption of each

particle striking z_2 is appropriate, provided that z_2 is carefully chosen. If we are considering, for example, glass beads with terminal velocity 10 cm s^{-1} in flow over a short grass surface, choice of $z_2 = z_0$ is reasonable. Even though $\sigma_w(z_0)$ is probably greater than the terminal velocity, we expect the particle to be absorbed because $\tau_L(z_0)$ is small.

A more difficult absorption boundary condition arises when the admixture may react chemically with the surface (e.g., ozone diffusing to a bare soil). Such situations have not been considered herein.

Consideration will now be given to the choice of $w_L(t_H)$, the Lagrangian vertical velocity for a particle at the reference height H. Except at the ground, we have chosen that there be no preference towards upward or downward movement for an individual fluid element, so that

$$\overline{w_L}(t_H) = 0.$$

It would therefore be possible to form $w_L(t_H)$ from a record of $w(H, t)$ which has had its time axis scaled to account for the ratio $\tau(H)/\tau_L(H)$, (perhaps by replaying a magnetic tape at a particular speed). We would hope that the spectral density and autocorrelation function for $w_L(t_H)$ thereby obtained would approximate those observed by actually following a particle.

In homogeneous turbulence, however, the rate of diffusion is not very sensitive to the exact form of the autocorrelation function (Pasquill, 1974), maximum sensitivity being for a diffusion time about equal to τ_L. We have therefore formed $w_L(t_H)$ by applying an RC filter (RC = $\tau_L(H)$) to the signal from a random voltage generator†. The spectral density of the unfiltered signal is independent of frequency out to a very high frequency F_G which is chosen such that

$$F_G \gg \frac{1}{2\pi \mathrm{RC}} = f_0$$

where f_0 is the half-power frequency of the filter. It may be shown that the autocorrelation function of $w_L(t_H)$ is

$$\overline{w_L(t_H)\, w_L(t_H + \xi)} \,/\, \overline{w_L^2} = \exp\left(-\xi/\tau_L(H)\right)$$

and that

$$w_L(t_H + \Delta t_H) = w_L(t_H) \exp\left(-\Delta t_H/\tau_L(H)\right) + \text{random variable}$$

so that the velocity series is similar to that used by Hall and Reid. The frequency distribution of the random voltage generator is approximately Gaussian, with zero mean; however, the distribution is truncated at ± 10 V, corresponding to a maximum turbulent velocity.

In order to minimise the computer time required to calculate a trajectory, in practice RC is reduced in relation to $\tau_L(H)$ by

† Hewlett-Packard Model 3722A; Hewlett-Packard, Palo Alto, California 94304, U.S.A.

$$\frac{\mathrm{RC}}{\tau_L(H)} = \frac{\Delta t_c}{\Delta t_H}$$

where Δt_c is the time taken by the computer to perform all the calculations for each timestep Δt_H.

In order to calculate a particle trajectory, the procedure is as follows:

Divide the z_* axis into layers of equal thickness Δz_* centered at $z_*(I) = (I - 1/2)\Delta z_*$. For each $z_*(I)$ calculate the corresponding $z(I)$, and store the values

$$\Delta x(I) = u(z(I)) \frac{\tau_L(z(I))}{\tau_L(H)} \Delta t_H.$$

Then release the particle, and in each timestep Δt_H calculate

$$\begin{aligned} \Delta z_* &= w_L(t_H)\Delta t_H \\ \Delta x &= \Delta x(I) \end{aligned} \tag{2}$$

where I is obtained from the instantaneous value of z_*. Should z_* reach 0 ($z = z_2$), the particle is absorbed (sink) or allowed to continue its motion in an image system with $z_* < 0$ (reflection).

In choosing a value for the timestep Δt_H, there are two considerations. The ratio $(\Delta t_H/\tau_H)$ need not be infinitely small, as it may be shown (Batchelor, 1949) that the higher the frequency of the motion, the smaller the contribution (in relation to lower frequencies) to the rate of turbulent dispersion. The larger we choose Δt_H, the smaller the computing time required to follow a particle a distance X. But unless $\Delta t_H \ll \tau_L(H)$, the timescale of the digitized time series is effectively increased over that of the analog time series. This is because the minimum time of correlation is Δt_H whereas in the analog series, samples persisting for times less than Δt_H occur.

We have generally used $\Delta t_H/\tau_L(H) \simeq 0.1$. No obvious differences occurred when a much smaller ratio was chosen. We did not systematically study the effect of reducing the timestep/timescale ratio.

Finally, it is worth noting that the use of Equations (2) to calculate particle trajectories is consistent with the hypothesis that particle motions exhibit Lagrangian similarity along the z axis;

$$w_L(t_H) = \frac{\mathrm{d}z_*}{\mathrm{d}t_H}$$

is a stationary random function of t_H.

3. Ensemble Experiments

The following discussion applies to calculation of the concentration distribution arising from a continuous source, but the trajectory-simulation method is readily able to deal with instantaneous-source problems.

Consider a continuous line source of strength 1 particle per unit crosswind length

per second at $x = 0$, and a detector downstream at $x = X$. Given the ability to calculate a trajectory $z_*(x)$, one may perform an ensemble of NP experiments in each of which a particle is followed from $x = 0$ to $x = X$. Each time a particle passes X in layer I

$$(I - 1)\Delta z_* < z_*(X) < I\Delta z_*$$

the count $N(I)$ in that layer is increased by 1. Then after all NP particles have been released

$$\frac{N(I)}{NP} = \text{time average count per second}$$
$$= \bar{F}_x(X, z)\Delta z(I)$$

where $\bar{F}_x(X, z)$ is the time average horizontal flux density, and $\Delta z(I)$ is the depth of the Ith layer,

$$\Delta z(I) = \frac{\tau_L(z(I))}{\tau_L(H)}\Delta z_*.$$

Since $\bar{F}_x(X, z) = u(z)\bar{c}(X, z)$, the time average concentration is obtained.

We may also write

$$\frac{N(I)}{N} = \bar{F}_{*_x}(X, z_*)\Delta z_*$$
$$= \left[u(z(z_*))\frac{\tau_L(z(z_*))}{\tau_L(H)}\right]\bar{c}_*(X, z_*)$$
$$= v_*(z_*)\bar{c}_*(X, z_*)$$

where $\bar{c}_*(X, z_*)$, v_*, and $\bar{F}_{*_x}$ are the concentration, horizontal velocity, and horizontal flux density in the (x, z_*, t_H) system. It follows that

$$\bar{c}_*(X, z_*) = \bar{c}(X, z).$$

The concentration field due to a plane source of spatially uniform strength may be considered as a superposition of the fields of elementary line sources. We regard a plane source of length XM cm as consisting of XM line sources each 1 cm in downwind width and emitting 1 particle per trial. The trajectory of the entire plane $z_*(x)$ is then calculated as if it were a single particle, and each time 1 cm of the plane passes the collection point X, a count of 1 particle is recorded in the layer (I) in which $z_*(X)$ lies. When the farthest upstream 1 cm has passed X, a new plane is released. We are therefore simultaneously performing an ensemble experiment for each of the XM line sources. The spatial correlation arising by treating the whole plane as one particle is unimportant. After the release of NP planes, we have NP independent trial trajectories from each line source.

It is worthwhile to point out that in the case of a passive tracer diffusing in the neutral surface layer, the count $N(I)/NP$ (i.e., the distribution of the values of

particle height at given x) is independent of u_*, because

$$\sigma_w \propto u_*$$

$$u \propto u_*$$

$$\tau \propto 1/u_*.$$

The vertical and horizontal steps Δz, Δx are affected equally by a change in the choice of u_* (and are independent of u_* if the timestep is kept in fixed proportion to the timescale). The number of timescales elapsed in travelling a distance δx at a height near z, $(\delta x/u(z))/\tau_L(z)$ is independent of u_*. Therefore, for a continuous source of strength Q the normalised horizontal flux density $\bar{u}(z)\bar{c}(z)/Q$ is independent of u_* (but not independent of the source geometry, roughness and displacement heights). If u_* doubles, $\bar{u}(z)$ is doubled and $\bar{c}(z)$ is halved.

Experimental values of σ_w/u_* in neutral stratification show variability in time and between locations, some of which may be ascribed to the difficulty of the measurements or to lack of suitable experimental conditions. To the extent that σ_w/u_* truly varies, one cannot expect the normalisation

$$\bar{u}\,\bar{c}/Q \quad \text{(or equivalently } u_*\,\bar{c}/Q\text{)}$$

to lead to a universal concentration profile, but it remains a very useful technique.

In the case where the source is continuous, conservation of mass requires

$$\frac{\partial}{\partial x}\bar{F}_x(x, z) = -\frac{\partial}{\partial z}\bar{F}_z(x, z)$$

so that $\bar{F}_z(X, z)$ may be determined given $\bar{F}_z(X, z_2)$ and the divergence of the horizontal flux at all heights. As a consequence of our approximation that $u(z)$ is time independent, the following symmetry occurs if the plane source extends without break to X and the surface (z_2) is a reflector. Consider the divergence of the horizontal flux between X and $X + 1$; refer to Figure 1. On average, for every particle which originates from the first line source upwind and passes $X + 1$ between z and $z + \Delta z$, another parallel trajectory originates from the 2nd line source upwind and crosses X between z and $z + \Delta z$. Therefore these two particles make no contribution to the flux divergence. By extension of this reasoning, it may be shown that the divergence of the horizontal flux is entirely due to the departure past $X + 1$ of particles from the farthest upstream 1 cm which are not 'balanced' by a corresponding arrival at X (whence if the plane is infinitely long, there can be no divergence of horizontal or vertical fluxes).

We therefore keep a special counter $NF(I)$ which is incremented each time the last 1 cm of the plane arrives in the corresponding layer. Then given $F_z(X, z_2)$ (1 cm^{-2} s^{-1} for source at $z = z_2$, 0 otherwise) it is straightforward to calculate $\bar{F}(X, z)$. For a source at ground

$$\bar{F}_z(X, z(I)) = \frac{\Sigma^{\text{all } J} NF(J) - \Sigma_{J=1}^{I} NF(J)}{\Sigma^{\text{all } J} NF(J)}$$

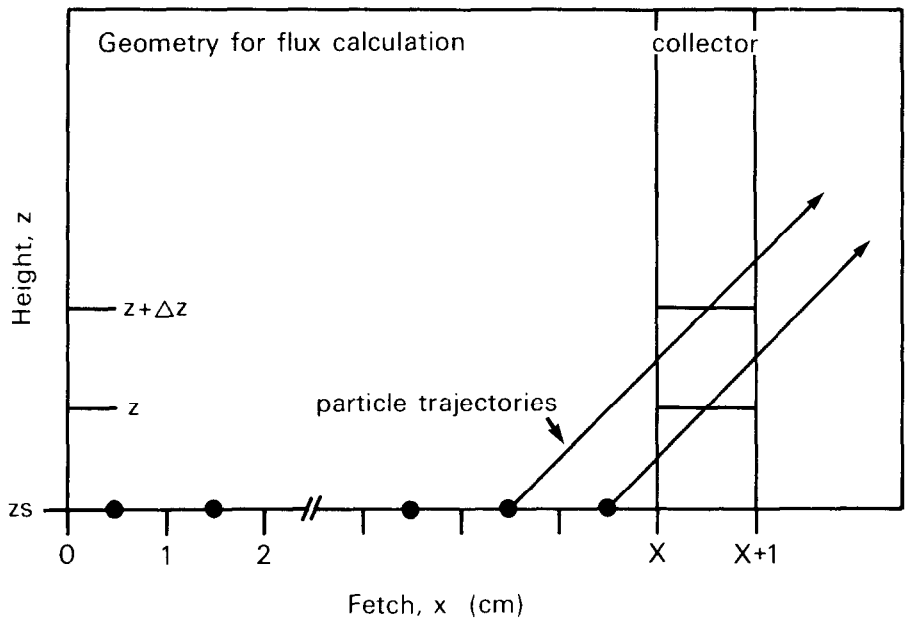

Fig. 1. Geometry illustrating the symmetry employed in calculating the vertical flux. The source extends upstream from $x = X$ to $x = 0$, and emits 1 particle per cm of its length. Consider particles entering and leaving the box defined by X, $X + 1$, z, $z + 1$ through the faces at X, $X + 1$. On average, for every particle emitted by the first upwind line source which passes through the box and leaves through the $X + 1$ face, another emitted by the second line source upwind enters through the front face at X. The two trajectories shown balance each other and contribute nothing to the divergence of the horizontal and vertical fluxes.

from which it may be deduced that the upward flux density at $z(I)$ is equal to the fraction of the particles released from the farthest upstream 1 cm of the plane which pass X above $z(I)$. Thus $\bar{F}_z(X, z)$ may be interpreted as a measure of the height to which material is being transported.

4. Tests of the Trajectory-Simulation Method in Special Cases where Analytical Solutions are Available

4.1. Homogeneous turbulence

A major advantage of the trajectory-simulation method is that the relationship of flux to mean gradient is automatically correct to the degree that the time and velocity scales of individual fluid element velocities are correctly simulated. This will be demonstrated for the case of diffusion in homogeneous turbulence. The concentration at the downwind edge of a long plane source of marked fluid elements in the absence of any barrier will be considered.

The concentration distribution downwind of a line source in homogeneous turbulence has been observed to be very close to Gaussian in form for ratios of

travel time to timescale t/τ_L ranging from near zero to much greater than 1 (Batchelor, 1949). Taylor (1921) gave an exact expression for the second moment of the concentration distribution (without assumptions as to the actual distribution). If the marked fluid elements are released at $t = 0$, $x = z = 0$ into a flow with Eulerian velocity field $(u, w(t))$, then the mean-square departure from $z = 0$ at a later time t is

$$\overline{z^2}(t) = 2\sigma_w^2 \int_0^t (t - \xi) R_L(\xi)\, d\xi. \tag{3}$$

The concentration at the downwind edge of a plane source may be obtained by adding together the Gaussian profiles for a large number of elementary line sources. For the contribution from the line source of width Δx a distance x from the source, the diffusion time is

$$t = x/u$$

and

$$\Delta\bar{c}(z) = \frac{\Delta x}{\sqrt{2\pi}\, u\, (\overline{z^2})^{1/2}} \exp\left(-z^2/2\overline{z^2}\right)$$

where $\overline{z^2}(t)$ is obtained from Equation (3) using

$$R_L(\xi) = \exp\left(-\xi/\tau_L\right)$$

corresponding to the autocorrelation function for RC-filtered Gaussian noise.

The contribution of each line source to the total vertical flux may be obtained by differentiating the expression for $\Delta\bar{c}(z)$ with respect to z and multiplying by the diffusivity (which is a function of the diffusion time x/u as will be discussed later).

In homogeneous turbulence Equations (1) reduce to

$$\Delta z = \Delta z_* = w_L(t)\Delta t$$

$$\Delta x = u\Delta t.$$

Figure 2 compares the solution of the trajectory method and the summation of the line-source analytical solutions, for a 100 m fetch and:

$$u = 100 \text{ cm s}^{-1}$$

$$\sigma_w = 25 \text{ cm s}^{-1}$$

$$\tau_L = 1 \text{ s}.$$

The agreement is excellent, both for concentration and vertical flux. Also plotted is the concentration profile obtained using a constant-K solution to the diffusion equation for each line source,

$$\Delta\bar{c}(z) = \frac{\Delta x}{\sqrt{2\pi}\, u \sqrt{2Kt}} \exp\left[-z^2/4Kt\right]$$

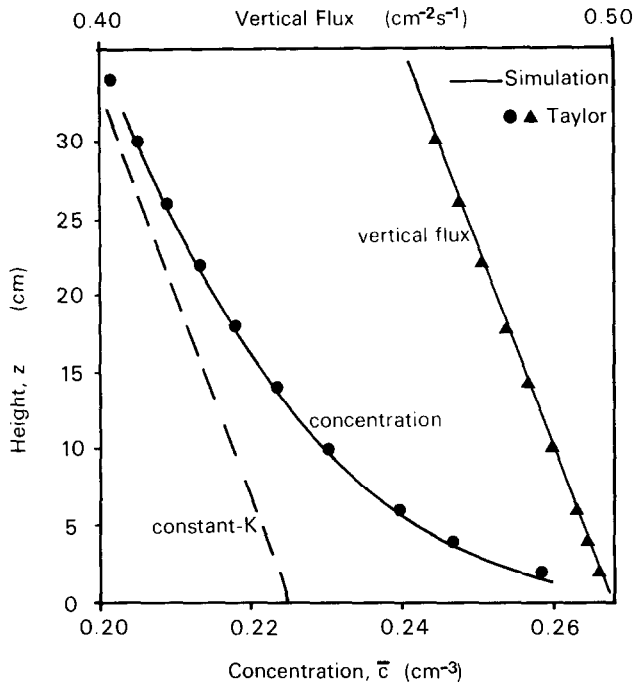

Fig. 2. Homogeneous turbulence. Prediction of the trajectory-simulation method for concentration and vertical flux at the downwind edge of a 100 m long plane source at $z = 0$ in homogeneous turbulence with length scale 25 cm, time scale 1 s, longitudinal velocity 100 cm s^{-1}. Source strength 1 cm^{-2} s^{-1}. The points labelled 'Taylor' were obtained by a superposition of the Gaussian solutions for each of a large number of elementary line sources placed side by side to construct the 100 m plane source: for each line source Taylor's expression for the second moment was used in the Gaussian solution. If a Gaussian solution with constant eddy diffusivity is used for each line source, the curve labelled 'constant-K' results.

where

$$K = \sigma_w^2 \tau_L = \sigma_w^2 \int_0^\infty R_L(\xi)\, d\xi.$$

Taylor's result, Equation (3), may be shown to imply that in fact

$$K = \sigma_w^2 \int_0^t R_L(\xi)\, d\xi$$

$$< \sigma_w^2 \tau_L \quad \text{for small } t.$$

It is therefore no surprise that the constant-K solution underestimates the concentration gradient near the source, where the total concentration has a large contribution from the elementary line sources immediately upwind. For the material

from nearby line sources, the closure relation

$$\bar{F}_z = -\sigma_w^2 \tau_L \frac{\partial \bar{c}}{\partial z}$$

is not correct.

4.2. Turbulence with power law wind and diffusivity profiles

It is also possible to compare the trajectory-simulation method with solutions to the diffusion equation for inhomogeneous turbulence. Philip (1959) gave a solution to the diffusion equation

$$u \frac{\partial \bar{c}}{\partial x} = \frac{\partial}{\partial z}\left(K \frac{\partial \bar{c}}{\partial z}\right)$$

with

$$u = u_1 \left(\frac{z}{z_1}\right)^m \qquad K = K_1 \left(\frac{z}{z_1}\right)^n$$

and surface boundary condition

$$\bar{F}_z(x, 0) = \left(-K \frac{\partial \bar{c}}{\partial z}\right)_{z=0} = 1 \quad \text{for} \quad x > 0$$

i.e., a ground-level source extending downstream from $x = 0$. Because the timescale at the source height is small, most of the material seen at the observation point will have been travelling for a time which is long compared to $\tau_L(zs)$*. Also, for a long fetch of source (large x), one would expect the concentration gradient to change only slowly along the vertical axis. We therefore expect Philip's K-theory solution to give correctly the concentration profile resulting from a long plane source at ground in a system with

$$\sigma_w = \text{constant}$$

$$\tau_L(z) \propto K(z) \propto z^n.$$

Diffusion in this artificial system may be simulated by writing

$$\frac{\tau_L(z)}{\tau_L(H)} = \frac{K}{K(H)} = \left(\frac{z}{H}\right)^n$$

and employing Equations (1). Figure 3 compares the solution thereby obtained with the analytical solution, for a 320 m long plane source and:

$$\begin{aligned} H &= 300 \text{ cm} \\ u(H) &= 500 \text{ cm s}^{-1} \\ K(H) &= 3000 \text{ cm}^2 \text{ s}^{-1} \\ \sigma_w &= 31 \text{ cm s}^{-1} \qquad (\tau_L(H) = 3.12 \text{ s}) \\ m &= 1/7 \\ n &= 6/7. \end{aligned}$$

* where zs = source height.

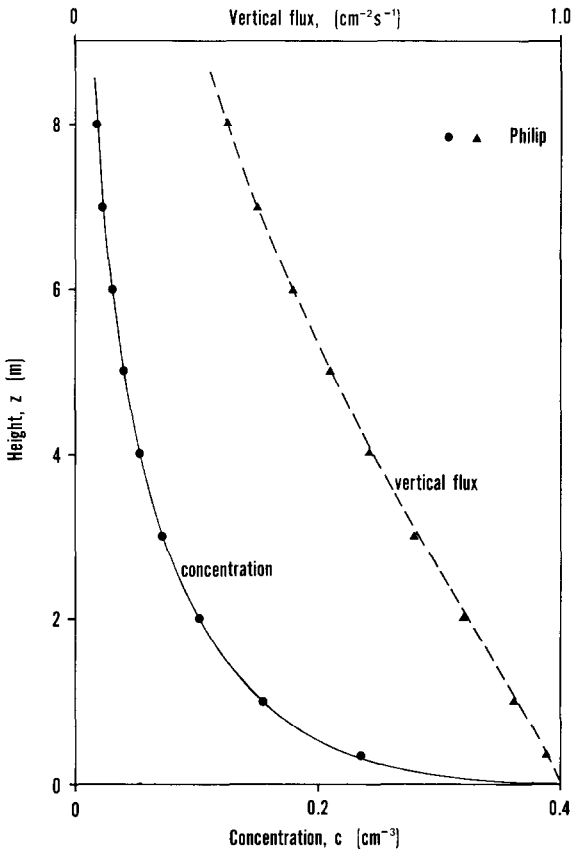

Fig. 3. Turbulence with power-law profiles of windspeed and eddy diffusivity. Prediction of the trajectory-simulation method and Philip's analytical solution for concentration and vertical flux at the downwind edge of a 320 m long plane source at ground in turbulence with $u \propto z^{1/7}$ and $K \propto z^{6/7}$ ($\tau_L \propto z^{6/7}$). The source strength is 1 $cm^{-2}\ s^{-1}$.

There is excellent agreement between the two solutions. It is possible to obtain the same profile of $K(z)$ by a different choice of σ_w and $\tau_L(H)$, (e.g., $\sigma_w = 100$ cm s^{-1}, $\tau_L(H) = 0.30$ s). Such an alternative choice, in which the particle trajectories are very different, leads to insignificant alteration in the concentration profile predicted by the simulation method. Our solutions are insensitive to modest changes in σ_w and τ_L which preserve $K = \sigma_w^2 \tau_L$ ($\sigma_w \to \beta\sigma_w$, $\tau_L \to \tau_L/\sqrt{\beta}$ where $\beta < 10$). No study of the limit to this insensitivity has been undertaken.

4.3. The neutral surface layer

For a plane source of infinite upwind extent at ground level, the vertical flux is independent of height, and one may integrate the closure relation

$$\bar{F}_z = -K\frac{\partial \bar{c}}{\partial z}$$

by assuming

$$K = a\sigma_w z$$

in the neutral surface layer. The resulting expression for the concentration is

$$\bar{c}(x, z) = \bar{c}(x, z_1) - \frac{\bar{F}_z}{a\sigma_w} \ln \frac{z}{z_1}. \tag{4}$$

Figure 4 shows the concentration and vertical flux-profiles predicted by Equations (1) for the downwind edge of a 320 m plane source of strength 1 $cm^{-2}\ s^{-1}$ at ground in the neutral surface layer, with

$u_* = 25$ cm s^{-1}
$z_0 = 0.1$ cm
$a = 0.5$
$\sigma_w = 31$ cm s^{-1}
$z_2 = zs = z_0$.

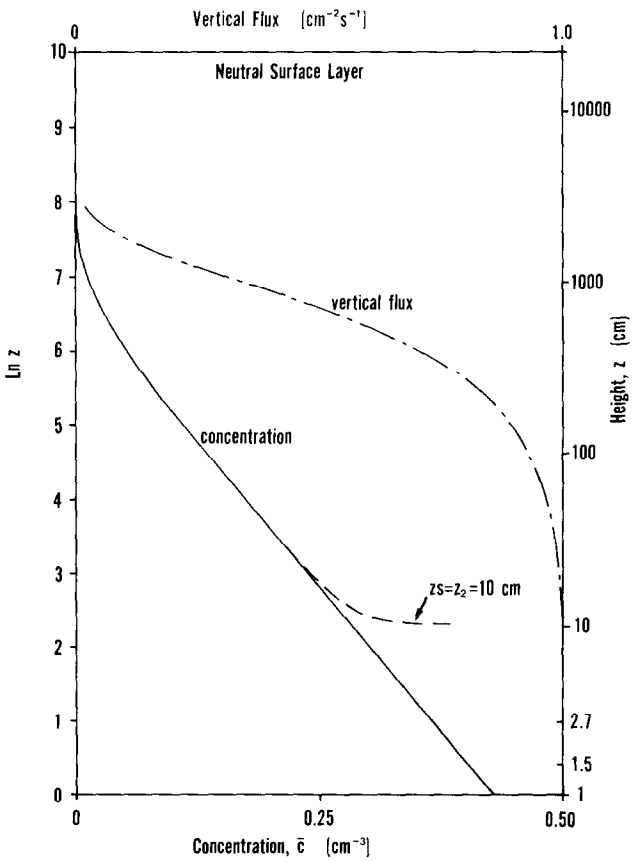

Fig. 4. Neutral surface layer. Prediction of the trajectory-simulation method for concentration and vertical flux at the downwind edge of a 320 m long plane source at ground in the neutral surface layer, with $u_* = 25$ cm s^{-1}, $z_0 = 0.1$ cm, source strength 1 $cm^{-2}\ s^{-1}$.

The straight-line portion of the concentration profile has slope

$$\frac{\Delta \bar{c}}{\Delta \ln z} = -\frac{1}{a\sigma_w}, \text{ in agreement with Equation (4).}$$

In consequence of the finite fetch, Equation (4) is not valid above the 'constant flux' region near the ground as is indicated by the trajectory-simulation technique. The dashed line is the solution when the source and reflection heights are chosen

$$zs = z_2 = 10 \text{ cm}.$$

It can be seen that except very close to the source, the solution is insensitive to the choice of zs, z_2.

5. Conclusion

A particle trajectory in inhomogeneous turbulence may be viewed as a motion in homogeneous turbulence in transformed coordinates. The motion in the transformed system may be numerically simulated using distance steps

$$\Delta z_* = w_L(t_H)\Delta t_H$$

$$\Delta x = u(z)\frac{\tau_L(z)}{\tau_L(H)}\Delta t_H$$

where z_* is the transformed height, related to real height z by the integral form of

$$\mathrm{d}z = \frac{\tau_L(z)}{\tau_L(H)}\mathrm{d}z_*;$$

t_H is transformed time, and $w_L(t_H)$ is a record of vertical velocity with the correct velocity scale (σ_w) and timescale ($\tau_L(H)$) for particle motion at height H.

Concentration profiles derived by calculating a large number of particle trajectories using this method have proven to be identical with analytical solutions for dispersion in homogeneous turbulence (in which case $\Delta z = \Delta z_*$), in turbulence with power-law profiles of windspeed and diffusivity, and in the neutral atmospheric surface layer. It may be concluded that this trajectory-simulation method is applicable to a wide variety of important diffusion problems. A comparison of predictions with experimental data for the atmospheric surface layer will be presented in another paper.

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