The simulation of particle motion in the atmosphere by a numerical random-walk model

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Summary

Of all the models of turbulent motion that are based on a random-walk technique, the simplest are ones which simulate individual particle trajectories. The accuracies of two such models are assessed by applying them to low-level diffusion in the atmosphere. It is found that one based on a Markov–Chain principle predicts particle concentrations over short and medium ranges which are consistent with observation. Calculations are extended to include dispersion in unstable conditions, and by postulating the dependence of several important turbulence parameters on $z/L$, it is possible to derive a physically realistic model.

1. Introduction

The diffusion equation has long been used to estimate the distribution of particles and pollutants in turbulent air, and its applications have been widely studied and are well established. There are occasions, however, when the method is unsatisfactory because, either the problem being investigated is complex and the equation has too many terms for an analytical solution to be found, or the statistical properties of individual particles are required which are unobtainable from the mean values of concentration that $K$-theory is able to predict. There are several accounts of attempts to overcome such difficulties by using a random-walk technique to simulate numerically particle motion. The procedure is simple, and, with the use of a computer, calculations can be performed in an acceptably short time. Each trajectory is reduced to a sequence of steps in each co-ordinate direction, representing the turbulent motion of a particle, from which a mean distribution can be obtained by averaging over many paths. With the position and velocity of each particle known at all times, it is possible to alter any parameters which may vary at every step, and study fairly complex problems without significantly increasing the number of calculations performed. The method is most suited to two-dimensional problems, and simple models have been developed to calculate the dispersion from a continuous point source of light tracer particles in the atmosphere (Thompson 1971), and in the flow of liquid down a channel (Sullivan 1971; Bugnarello and Jackson 1964). More detailed models based on a Markov–Chain principle have been used to study the statistical properties of Eulerian wind fluctuations close to the ground (Daniels and Jones 1970), and the effect of turbulence on the growth of droplets in a cloud (Jonas and Bartlett 1972). Although all these authors report useful results obtained from their models and in some cases good agreement with experimental data relating to their study, no assessment of the method has been made which compares the predicted downwind distribution of tracer particles from a low-level or ground-level source in the atmosphere with well-established observational results. It will be essential to take into account the behaviour of the particles as they come into contact with the solid boundary as well as defining their motion in the non-homogeneous flow above the surface. Simulations of long-range diffusion are in most cases excluded as it becomes impracticable to compute a sufficient number of paths to give statistically accurate results.
2. **Random-walk Models**

In order to simulate particle motion in the atmosphere by a sequence of steps $\Delta x_i$, $\Delta y_i$, $\Delta z_i$ made at time intervals of $\Delta t_i$ in the three co-ordinate directions, it will be necessary to define in some way the Lagrangian velocity $(u_i, v_i, w_i)$ experienced by the particle at each step, so that the important statistics of the motion, notably the correlation function $R(t)$, take realistic values. The displacement from the origin after $n$ steps is expressed by

$$(x, y, z) = \left( \sum_{i=1}^{n} u_i \Delta t_i, \sum_{i=1}^{n} v_i \Delta t_i, \sum_{i=1}^{n} w_i \Delta t_i \right).$$

For homogeneous turbulence, Taylor (1921) has shown that the variance of the displacement from a point source in one dimension is determined by the Lagrangian correlation function for the velocity component in that direction, and is given by

$$\bar{y}^2 = 2\sigma_v^2 \int_{0}^{T} \int_{0}^{t} R(\xi) d\xi dt$$

where $T$ is the time of flight of the particles and $\sigma_v$ the standard deviation of the velocity fluctuations. The time scale of the Lagrangian motion is

$$\tau_L = \int_{0}^{\infty} R(\xi) d\xi.$$

If $\tau_L$ varies with the position of the particle, Eq. (1) does not apply, and since, in all but the simplest cases, the equations defining the displacement are hard to solve analytically, numerical simulation methods will have to be used.

Most random-walk models divide naturally into two groups:

(a) Those, greatly simplified, using a large time interval which defines the broad-scale characteristics of turbulent motion; and

(b) Those, more detailed, using a small time interval with a correlation between velocities at successive steps -- a Markov-Chain model. Assuming for the moment that the particle velocities in each co-ordinate direction vary independently, it is only necessary to consider models which simulate the fluctuating component $v$ in one dimension, where $\bar{v} = 0$.

(a) A typical large-step model (I) takes time steps of duration $\Delta t$ and particle velocities, constant throughout each step, which are chosen randomly from a Gaussian distribution with mean zero. The correlation function for the model can be shown to be

$$R(t) = \begin{cases} 1 - t/\Delta t & t < \Delta t \\ 0 & t \geq \Delta t \end{cases}$$

and the time scale

$$\tau_L = \int_{0}^{\infty} R(\xi) d\xi = \Delta t/2.$$

Substituting into Eq. (1) the variance of particle spread in homogeneous turbulence is

$$\bar{y}^2 = 2\sigma_v^2(T\tau_L - \frac{3}{2} \tau_L) \quad T \gg 2\tau_L$$

which tends to $2\sigma_v^2T\tau_L$ for large $T$.

(b) In order that the scale of motion should remain relatively large, models with a short time step introduce a correlation between velocities during successive steps. Such a model (II) is conveniently based on a Markov assumption that the velocity during step $i+1$ is given by

$$v_{i+1} = \alpha v_i + r_i$$

(4)
where \( \alpha \) is a constant and \( r_i \) is a random variable with mean zero and standard deviation \( \sigma \), which is independent of all the \( v_i \). This is no doubt an over simplification as it ignores the fact that the velocity at any time depends not only on the velocity during the previous step, but probably also on the rate of increase of velocity and on its sign (downward and upward moving particles may have different statistics). Using Eq. (4) the correlation between velocities separated by \( n \) steps is

\[
R(n\Delta t) = \frac{v_i v_{i+n}}{v_i^2} = (\alpha^n v_i^2 + \alpha^{n-1} v_i r_i + \ldots + \alpha v_i r_{i+n-1}) / v_i^2 = \alpha^n
\]

since all the \( r_i \) are independent of the \( v_i \). Clearly this leads to \( R(t) \) taking a power-law form at the times \( 0, \Delta t, 2\Delta t, \ldots \) approximating to \( \exp(-t/\tau_L) \) when \( \Delta t \ll \tau_L \) and

\[
\alpha = \exp(-\Delta t/\tau_L) \tag{5}
\]

Taking variances of both sides of Eq. (4)

\[
\sigma_v^2 = \alpha^2 \sigma_v^2 + \sigma_r^2
\]

which gives

\[
\sigma_r = \sigma_v \sqrt{1 - \alpha^2} \tag{6}
\]

Substituting the exponential correlation function into Eq. (1), the variance of particle spread is

\[
y^2 = 2\sigma_r^2 \{ T\tau_L - \tau_r^2 [1 - \exp(-T/\tau_L)] \}
\]

which only differs significantly from Eq. (3) when \( T \) is small compared with \( \tau_L \).

These two models which lead to the same dispersion of particles over large distances in homogeneous turbulence, will be applied to diffusion downwind of a low-level source in a thermally neutral atmosphere. The time scale is known to change rapidly with height and the models will be adapted to inhomogeneous motion in a simple manner as follows:

(i) Calculations are restricted to the downwind \((x)\) and vertical \((z)\) dimensions to give values of crosswind integrated concentration from a point source, or, equivalently, point concentration from a line source.

(ii) The mean vertical velocity \( \bar{w} \) is zero, and the mean horizontal velocity is given by the neutral logarithmic profile, \( \bar{u} = (u_*/k) \ln z/z_0 \) where \( k \) is von Kármán's constant, taken to be 0.4, and \( u_* \) is the friction velocity.

(iii) A simple time correlation between \( u \) and \( w \) is introduced by letting the fluctuating component of the horizontal wind \( u' \) be of constant magnitude 2.2\( u_* \).

\[
u = \bar{u} \pm 2.2u_* \tag{7}
\]

The sign in Eq. (7) is opposite to that of \( w \) with probability \( P \), and on all other occasions is positive or negative at random. \( P \) is chosen so that the correlation takes its normally observed value of \(-0.25\) in neutral stability. It is felt that such a simplification is justified since the effect of \( u' \) on the dispersion of particles in the lateral or vertical directions, although found not to be negligible, is not of major importance.

(iv) In neutral or near-neutral conditions the Eulerian scale of motion \( l_E \) is proportional to the height above the ground, and hence the time scale is \( \tau_E = l_E/\bar{u} \propto \tau/\bar{u} \). As direct Lagrangian measurements are not easily made it is usual to assume that the ratio of the two time scales is a constant,

\[
\tau_L/\tau_E = \beta \tag{8}
\]
which has a probable neutral value between 3 and 5 (Hay and Pasquill 1959). The Langrangian time scale can now be written

$$\tau_L = \frac{cz}{\bar{u}}$$  \hspace{1cm} (9)$$

where $c$ is a constant.

(v) Numerous observations in the atmospheric boundary layer have shown that the standard deviation of the vertical velocity fluctuation is given by

$$\sigma_w = 1.3u_*$$

(vi) All particles are reflected with reversed vertical velocity off a surface a small distance $z_s$ above the ground. Alternatively the boundary condition can be modified by absorbing with a given probability any particle striking the reflecting surface, to account for sedimentation or surface absorption.

$x, z, u, w, t$ and $\tau_L$ are now replaced by the dimensionless quantities $X, Z, U, W, T$ and $T_L$ by dividing velocities by $u_*$ lengths by $z_0$ and times by $z_0/u_*$. The large-step model (I) has a correlation function given by Eq. (2) and steps of duration $2T_L$ during which a constant vertical velocity $W$ independent of the velocities during the previous steps, carries the particle up or down. Each step is

$$\Delta Z = 2cZW/\bar{U} = 2.6cZR/\bar{U}$$

$$\Delta X = 2cZU/\bar{U}$$  \hspace{1cm} (10)$$

where $R$ is a normally distributed random variable with zero mean and unit standard deviation.

The Markov–Chain model (II) has steps

$$\Delta Z = \delta cZW/\bar{U}$$

$$\Delta X = \delta cZU/\bar{U}$$

where $\delta = \Delta T/T_L$ is the measure of the step size relative to the scale of turbulence, and the vertical velocity $W$ at each step is calculated from Eq. (4) using Eqs. (5), (6), (9) and (10).

It only remains to assign a value to $c$, the measure of the scale of turbulence, for both models to be used to make numerical estimates of atmospheric diffusion. In a summary of recent measurements of Eulerian turbulence spectra, Pasquill (1972) finds that the parameter $\lambda_m/\pi$ takes a value between 2 and 4 where

$$\lambda_m = \bar{u}/n_m$$  \hspace{1cm} (11)$$

and $n_m$ is the frequency at which the vertical velocity spectrum has a maximum.

The exponential correlation function has the spectrum

$$nF(n) = \frac{2}{\pi(a + 1/a)} \quad a = 2\pi n\tau_E$$

with a maximum at $a = 1$. This gives

$$\tau_E = \left(\frac{\lambda_m}{2\pi \bar{u}}\right) \frac{z}{\bar{u}}$$

and from Eqs. (8) and (9) it follows that $c$ should lie between 1 and 3.3 with a probable value around 2. The fact that the range of values is so wide merely reflects the difficulties encountered when measuring Lagrangian properties. Rather than assign a definite value to the scale of turbulence, a value for $c$ will be found which gives a satisfactory simulation.
of diffusion in the atmosphere over a fixed distance (100m), and with this value the predicted diffusion over longer distances (up to about 500m) can be compared with typical experimental results.

3. Numerical results

All numerical simulation models require a sequence of numbers chosen randomly from a Gaussian distribution with zero mean and unit standard deviation. A pseudo-random number generator based on the relation

$$r_{i+1} = k r_i \text{ (mod } m)$$

with $k = 2^{19} + 3$ and $m = 2^{37}$ was used in all the following calculations. The set of numbers generated in this way is uniformly spread over the interval between 0 and 1, and the transformation to the required distribution is now straightforward. Several statistical checks on the numbers were performed including a simulation of one-dimensional homogeneous turbulence for which the particle dispersion after a time $T$ was compared with the expected distribution with a standard deviation given by Eq. (1). Taking ten sets of 1000 paths and $T = 100 T_L$, $\chi^2$ tests were satisfactory at the 5\% level, and it was concluded that the method of random-number generation was suitable for these purposes.

(a) Diffusion in neutral conditions

Using model I for the diffusion of material from a ground-level source, particle concentration in arbitrary units is calculated as a function of the height above the ground at a fixed downwind distance $X = 3200$, when the source height and $Z_s = 8$ and for $c = 2, 3, 4$ and 6 (Fig. 1). Compared with the observed profile over rough downland ($z_0 = 3cm$), the results are poor; the profile shape has an excessive peak close to the ground, and the cloud height, defined by the point where the concentration falls to one tenth of its maximum value, is considerably lower than expected. Variation of the height of the reflecting surface

![Figure 1. Concentration in arbitrary units at a dimensionless distance 3200 downwind of a line source calculated using model I. Source height and $Z_s = 8$ and the turbulence parameter $c$ takes the values 2, 3, 4 and 6.](image-url)
has little effect on the results, and \( c \) has to be increased well outside its expected range of 1 to 3-3 to give sufficient vertical diffusion.

An application of model II under the same conditions and with \( \delta = 0.125 \), leads to realistic particle trajectories (Fig. 2) and much improved profile shapes (Fig. 3). If \( c = 2-4 \), the cloud height 100m downwind of a source over a terrain with \( z_0 = 3 \text{cm} \) takes the accepted value of 10m. By observing the effect of gradually increasing the step duration \( \Delta T \) of model

![Figure 2](image)

Figure 2. Example of particle trajectories using a Markov–Chain model.

II until it reaches \( 2T_L \), the step duration of model I, while at the same time reducing the velocity correlation between successive steps, it is possible to deduce the reason for the large discrepancies observed between the two models, which, in homogeneous turbulence, predict the same particle dispersion. It appears that close to the reflecting boundary, a large-step model fails to account for the rapidly changing scale of turbulence with height.

![Figure 3](image)

Figure 3. Concentration in arbitrary units at a dimensionless distance 3200 downwind of a line source calculated using model II. Source height and \( Z_r = 8 \), \( \delta = 0.125 \) and the turbulence parameter \( c \) takes the values 2, 2-4, 3 and 4.
close to the ground, and with no correlation between velocities separated by an interval of time longer than $2T_L$, there are fewer sustained particle movements in one direction which enable an escape from the surface to be made. The discrepancies become far less for the diffusion from elevated sources, when particle trajectories remain predominantly well above the boundary.

![Cloud height vs downwind distance](image)

Figure 4. Cloud height in neutral conditions downwind of a line source calculated using model II (crosses) and compared with typical values observed over rough downland (broken line).

Taking $c = 2.4$, it is now possible to extend the diffusion calculations of model II to give cloud heights at downwind distances up to $X = 16,000$ (500m) and a comparison with estimates based on observational data over rough downland (Pasquill 1961) can then be made (Fig. 4). The results compare favourably for $X < 10,000$ (300m), but appear a little too small beyond this distance. Model I still underestimates particle diffusion at longer ranges (for example, the predicted cloud height is only half of the observed value when $X = 16,000$ (500m)); many particles remain in the near-surface region, and the concentration peak, although less marked, is still unrealistic.

(b) Diffusion in unstable conditions

No diffusion model can be considered satisfactory unless it can account for the large changes in dispersion rate that are observed as the atmosphere becomes thermally stratified. It seems acceptable, as a simplifying approximation, to leave unaltered the assumptions on which model II has so far been based and merely modify the values of $u/u_*$, $\sigma_w/u_*$, $\sigma_u/u_*$ and $c$ used in the calculations to take into account the more intense and prolonged velocity fluctuations which are caused by convective elements in the atmosphere. Many turbulence measurements have been made which record these parameters as functions of $z/L$, where $L$ is the Monin–Obukhov length. The following results for unstable conditions will be used:

(i) The horizontal wind velocity defined by

$$\frac{du}{dz} = \frac{u_*}{kz} \left(1 - \frac{16z}{L}\right)^{-\frac{1}{4}}$$

gives the best fit to observational data (Businger et al. 1971).

(ii) Dimensional analysis predicts that

$$\frac{\sigma_w}{u_*} = \frac{a}{k^{\frac{1}{2}}} \left(\frac{z}{L}\right)^{\frac{1}{2}}$$
for large $|z/L|$. Theory is born out by recent measurements by Caughey and Readings (1973) and Monji (1973) for values of $-z/L$ up to 100 which give $a$ equal to approximately 1.1. Other authors (e.g. Haughen et al. 1971; Monji and Businger 1972; McBean 1970) present data for $z/L$ in the range 0 to $-2$, and their results are used to determine the effect on the model of small deviations from neutral stability.

(iii) McBean gives the dependence of $\sigma_u/u_*$ on stability as $\sigma_u/u_* = 2.2 - 0.862/L$ for $z/L$ between 0 and $-5$. The relationship is extrapolated to some negative values of $z/L$ larger than $-5$, but since the effect of fluctuations of $u$ on particle dispersion is found to be small, no significant errors should result.

(iv) Pasquill (1972) finds that most turbulence measurements in unstable conditions indicate an increase in $\lambda_m/z$ (Eq. (11)) from its neutral value, but that estimates of its magnitude vary. At the same time it is thought that $\beta$ (Eq. (10)) decreases, leading to the conclusion that there may be no great change in the value of $c$. However, quite small changes can appreciably alter particle dispersion predicted by the model, and so it will again be necessary to find values which, when applied to diffusion over a fixed distance (100m), give cloud heights agreeing with observation. The calculations can then be extended to greater downwind distances.

**TABLE 1. Cloud height in metres, 100m downwind of a line source, for $c = 2.4, 4.0, 5.0$ and 6.0**

<table>
<thead>
<tr>
<th>$c$</th>
<th>2.4</th>
<th>4.0</th>
<th>5.0</th>
<th>6.0</th>
<th>Observation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutral</td>
<td>10</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>10</td>
</tr>
<tr>
<td>$L = -20m$</td>
<td>12</td>
<td>17</td>
<td>—</td>
<td>—</td>
<td>16</td>
</tr>
<tr>
<td>$L = -10m$</td>
<td>14</td>
<td>20</td>
<td>22</td>
<td>—</td>
<td>23</td>
</tr>
<tr>
<td>$L = -5m$</td>
<td>16</td>
<td>24</td>
<td>26</td>
<td>29</td>
<td>30</td>
</tr>
</tbody>
</table>

**TABLE 2. Cloud height in metres at distances of 100, 200, 300 and 500m downwind of a line source for $L = -20$, $-10$ and $-5m$**

<table>
<thead>
<tr>
<th>Distance</th>
<th>100m</th>
<th>200m</th>
<th>300m</th>
<th>500m</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>calc.</td>
<td>obs.</td>
<td>calc.</td>
<td>obs.</td>
</tr>
<tr>
<td>Neutral</td>
<td>10</td>
<td>10</td>
<td>19</td>
<td>18</td>
</tr>
<tr>
<td>$L = -20m$</td>
<td>17</td>
<td>16</td>
<td>25</td>
<td>30</td>
</tr>
<tr>
<td>$L = -10m$</td>
<td>22</td>
<td>23</td>
<td>40</td>
<td>44</td>
</tr>
<tr>
<td>$L = -5m$</td>
<td>29</td>
<td>30</td>
<td>60</td>
<td>63</td>
</tr>
</tbody>
</table>

For the Pasquill stability categories C ($L \approx -20m$), B ($L \approx -10m$) A ($L \approx -5m$) it is found that $c = 4.0, 5.0$ and 6.0 respectively gives cloud heights of 17, 22 and 29m (Table 1) 100m downwind of a line source, which approximate to estimates based on observational data over rough downland ($z_0 = 3cm$) given by Pasquill (1961). Extending the same calculations to 200, 300 and 500m and keeping $|z/L|$ less than 12, the results (Table 2) show some underestimation of cloud height in all instances. This could be caused by some assumptions made for the neutral case no longer being such good approximations in unstable conditions; there may be deviation from the linear dependence of the time scale on $z$ (Eq. (8)), and the Markov assumption may need to be modified to model convective elements. However, the results are in broad agreement with observation, and even with the simplifications made, small-step Markov-Chain models appear applicable in a wide range of meteorological conditions. No doubt it would be possible to improve on the results just obtained by modelling in more detail each parameter used; for example the value of $c$ could be defined as a function of $z/L$. However, the main drawback of the
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random-walk method in such cases is that the detailed structure of turbulence has to be specified, involving much more empiricism than is introduced into any K-theory model.

4. Conclusions

Two types of random-walk models which have been used to simulate turbulent motion, have been applied to the low-level diffusion of particle clouds in the atmospheric boundary layer. It is found that models that have a step length of the same order as the scale of turbulence do not predict sufficient vertical diffusion, and an excessive concentration peak is formed at the surface. If the step size is reduced and a correlation introduced between successive particle velocities, results can be obtained for neutral stability which compare favourably with observation. An extension to unstable conditions can be made if a suitable dependence of important turbulence parameters on L is postulated.

Although random-walk models can produce satisfactory results in well-defined conditions, much empiricism has been used which limits their application to more general problems. Their main advantage is that statistics of turbulent motion, which are not readily deduced from solutions to the diffusion equation, can be easily calculated. In practice, computing time restricts the application to one and two-dimensional simulations of particle trajectories over short or medium ranges.

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