CALCULATION OF PARTICLE TRAJECTORIES IN THE PRESENCE OF A GRADIENT IN TURBULENT-VELOCITY VARIANCE

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Abstract. Recent papers by Wilson *et al.* (1981b) and Legg and Raupach (1982) give methods for the calculation of particle trajectories in turbulence with a gradient in vertical velocity variance σ_w^2. However the two methods seem contradictory.

This paper demonstrates that in systems in which $l(\mathrm{d}\sigma_w/\mathrm{d}z)$ (where l is the length scale) varies only slowly with height z, the two methods give similar predictions, and indicates why this is the case. For a particular system in which the restriction on $l(\mathrm{d}\sigma_w/\mathrm{d}z)$ is not satisfied, it is shown that neither method is correct but that a simple modification of the method of Wilson *et al.* (1981b) gives reasonable predictions.

1. Introduction

Trajectory-simulation models of turbulent dispersion have been proven to be in precise agreement with analytical solutions in several simple systems, and in very good agreement with observations of dispersion in the atmosphere and the wind tunnel (Reid, 1979; Wilson *et al.*, 1981a, c; Legg, 1983). They are particularly suited to cases which have 'flux' boundary conditions (specified rate of emission) and which cannot easily be solved by solution of the equation of mass conservation. The velocity statistics proven by Taylor (1921) to be of paramount importance are correctly incorporated, and there is no necessity for a closure hypothesis (such as K-theory).

The trajectory-simulation method employs detailed information on the turbulence statistics. It is therefore likely to prove useful for the case of dispersion within the highly inhomogeneous turbulence which exists in flow through a plant or forest canopy. Within a canopy, there is a strong vertical gradient in the root-mean-square Eulerian vertical (z) velocity $\sigma_w = (\overline{w^2})^{1/2}$. Wilson *et al.* (1981b; hereafter WTK) showed that such a gradient in σ_w implies that a particle trajectory must be biased towards larger values of σ_w, according to their method with a velocity

$$\overline{w}_{\mathrm{WTK}} = l\,\frac{\mathrm{d}\sigma_w}{\mathrm{d}z}\ ,$$

where $l(z) = \sigma_w(z)\,\tau_L(z)$ is the Lagrangian length scale formed from the Lagrangian time scale of the vertical velocity $\tau_L(z)$. In several systems, this compensation was shown to lead to dramatic improvement in the predicted concentration profile, but in the case of diffusion within a corn canopy, for example, anomalies remained.

Legg and Raupach (1982; hereafter LR) have pointed out that a vertical gradient in σ_w in a horizontally homogeneous system is always associated with a vertical gradient in the pressure departure from hydrostatic equilibrium. A force must therefore be applied to a fluid element. By incorporating this force into the stochastic equation for the motion of a fluid element, Legg and Raupach derived a bias velocity

$$\overline{w}_{\mathrm{LR}} = \tau_L \frac{\mathrm{d}\sigma_w^2}{\mathrm{d}z} = 2l \frac{\mathrm{d}\sigma_w}{\mathrm{d}z} = 2\overline{w}_{\mathrm{WTK}}\,.$$

This paper investigates the apparent contradiction between the WTK and LR methods.

2. The WTK and LR Methods

The WTK method involves calculating trajectories in (x, z_*, t_H) coordinates, where the real height (z) and time (t) coordinates are related to the z_* and t_H coordinates by

$$\mathrm{d}z = \frac{\sigma_w(z)}{\sigma_w(H)}\,\frac{\tau_L(z)}{\tau_L(H)}\,\mathrm{d}z_* \tag{1a}$$

$$\mathrm{d}t = \frac{\tau_L(z)}{\tau_L(H)}\,\mathrm{d}t_H \tag{1b}$$

and distance steps on the z_* axis are calculated from

$$\Delta z_* = w_L(t_H)\Delta t_H + \overline{w}_*\Delta t_H\,. \tag{1c}$$

Here H is an arbitrary reference height, $w_L(t_H)$ is a record of velocity with statistics appropriate to motion at $z = H$, t_H is transformed time, and $\overline{w}_*$ is the bias velocity along the z_* axis. For further details, refer to WTK. The important point in the present context is that as a particle moves along the z_*-axis the image motion in z corresponds to an instantaneous adoption by the fluid element of the local value of the standard deviation of vertical velocity.

The LR method calculates trajectories in (x, z, t) coordinates using

$$\Delta z = w\Delta t(z) \tag{2a}$$

$$\Delta x = u(z)\Delta t(z) \tag{2b}$$

$$\Delta t = \mu\tau_L(z) \tag{2c}$$

where $\mu \ll 1$ and w is formed from a Markov chain:

$$w^{n+1} = \alpha w^n + \beta\sigma_w^{n+1} r^{n+1} + \gamma\overline{w}_{\mathrm{LR}}\,. \tag{3}$$

Here

$$\alpha = \exp(-\Delta t/\tau_L) \tag{4a}$$

$$\beta = (1 - \alpha^2)^{1/2} \tag{4b}$$

$$\gamma = 1 - \alpha \tag{4c}$$

$$\overline{w}_{\mathrm{LR}} = \tau_L \frac{\mathrm{d}\sigma_w^2}{\mathrm{d}z}$$

and r is a Gaussian random number with zero mean and unit variance.

The point to note is that the LR method imposes a memory of w as a whole, including a memory of σ_w and $\overline{w}_{\mathrm{LR}}$. By averaging Equation (3) over many velocity choices at or near height z^n, we obtain

$$\overline{w^{n+1}} - \alpha\overline{w^n} \approx \gamma\overline{w}_{\mathrm{LR}} \tag{4d}$$

and if we write $\overline{w^{n+1}} \approx \overline{w^n}$, then $\overline{w^n} \approx \overline{w}_{\mathrm{LR}} = \tau_L(\mathrm{d}\sigma_w^2/\mathrm{d}z)$.

For a sufficiently small choice of $\Delta t/\tau_L$, the trajectories calculated by the WTK method are equivalent to trajectories calculated in (x, z, t) coordinates using Equations (2), (3′), (4) (labelled WTK′ for convenience), where

$$q^{n+1} = \alpha q^n + \beta r^{n+1} \tag{3'a}$$

$$w^{n+1} = \sigma_w^{n+1} q^{n+1} + l\,\frac{\mathrm{d}\sigma_w}{\mathrm{d}z}\,. \tag{3'b}$$

Further, if $l(\mathrm{d}\sigma_w/\mathrm{d}z)$ changes only very slowly with height, WTK′ is negligibly altered by writing (WTK″):

$$s^{n+1} = \alpha s^n + \beta r^{n+1} + \gamma\tau_L\,\frac{\mathrm{d}\sigma_w}{\mathrm{d}z} \tag{3''a}$$

$$w^{n+1} = \sigma_w^{n+1} s^{n+1}\,. \tag{3''b}$$

There are two differences between LR and WTK″. The LR Markov chain is written in terms of w and uses bias velocity $\tau_L(\mathrm{d}\sigma_w^2/\mathrm{d}z)$ while the WTK″ Markov chain uses $s = w/\sigma_w$ and bias velocity $l(\mathrm{d}\sigma_w/\mathrm{d}z)$. The following argument indicates that these two differences may compensate for each other.

Equations (3″a) and (3″b) may be combined as

$$\frac{w^{n+1}}{\sigma_w^{n+1}} = \alpha\,\frac{w^n}{\sigma_w^n} + \beta r^{n+1} + \gamma\tau_L\,\frac{\mathrm{d}\sigma_w}{\mathrm{d}z}\,.$$

Now

$$\sigma_w^{n+1} \approx \sigma_w^n + w^n\Delta t\,\frac{\mathrm{d}\sigma_w}{\mathrm{d}z}$$

and $\Delta t \approx (1 - \alpha)\tau_L$, so that

$$w^{n+1} - \alpha w^n \approx \alpha(1 - \alpha)\frac{(w^n)^2}{\sigma_w^n}\tau_L\frac{d\sigma_w}{dz} + \beta\sigma_w^{n+1}r^{n+1} + \gamma\sigma_w^{n+1}\tau_L\frac{d\sigma_w}{dz}.$$

Average this equation over many velocity choices at or near height z^n. Assuming that $\overline{(w^n)^2} \approx (\sigma_w^n)^2$ (i.e. that the bias velocity is small with respect to σ_w),

$$\overline{w^{n+1}} - \alpha\overline{w^n} \approx \alpha(1 - \alpha)\sigma_w^n\tau_L\frac{d\sigma_w}{dz} + \gamma\sigma_w^{n+1}\tau_L\frac{d\sigma_w}{dz}$$

$$\approx \sigma_w^n\tau_L\frac{d\sigma_w}{dz}[\alpha(1 - \alpha) + \gamma]$$

where a term in $(d\sigma_w/dz)^2$ has been neglected. Now for small $\Delta t/\tau_L$, $\gamma + \alpha(1 - \alpha) \approx 2\gamma$. Hence

$$\overline{w^{n+1}} - \alpha\overline{w_n} \approx \gamma\tau_L\frac{d\sigma_w^2}{dz}.$$

This result is the same as that obtained from Equation (3), the LR method. Hence, under the restrictions of the preceding derivation, the WTK″ method has the same value for $\overline{w^n}$ as does the LR method, namely $\overline{w^n} = \tau_L(d\sigma_w^2/dz)$, even though the explicitly applied bias velocity $\overline{w}_{\mathrm{WTK}}$ is only half this value. The factor-of-two difference between $\overline{w}_{\mathrm{LR}}$ and $\overline{w}_{\mathrm{WTK}}$ is related to the distinction between formulation of the Markov chain in terms of w/σ_w or in terms of w.

We therefore expect the results of trajectory-simulation experiments following the WTK, WTK′, WTK″, and LR methods and performed using small $\Delta t/\tau_L$ to be similar for the restricted set of turbulence systems having slowly varying $l(d\sigma_w/dz)$ and bias velocity small with respect to σ_w. If these restrictions are not satisfied, we may expect markedly different predictions from each of the methods. This is confirmed in the following section.

3. Simulations

3.1. Comparison with Analytical Solution

The trajectory-simulation methods were used to calculate the concentration profile 100 m downwind of a line source of strength Q = 100 particles m^{-1} s^{-1} at $z = 0$ in turbulence with

$$\overline{u}(z) = 0.50\left(\frac{z}{z_1}\right)^{0.15} \qquad [\mathrm{m\,s^{-1}}]$$

$$\tau_L(z) = \left(\frac{z}{z_1}\right)^{0.15} \qquad [\mathrm{s}]$$

$$\sigma_w(z) = 0.30\left(\frac{z}{z_1}\right)^{0.5} \qquad [\mathrm{m\,s^{-1}}]$$

where $z_1 = 1$ m and the ground was treated as a reflector.

Figure 1 shows the analytical solution for the concentration profile using the diffusion equation with $K = \sigma_w^2(z)\,\tau_L(z)$ (see Pasquill, 1974) and trajectory-simulation results using the WTK″ and LR methods. The WTK′ method gave a result indistinguishable from WTK″. The predicted profile using Equation (3) with $\gamma = 0$ (no offset velocity included) is also shown. The LR prediction is superior to WTK″ very near the ground but at greater heights, there is little difference between the two solutions.

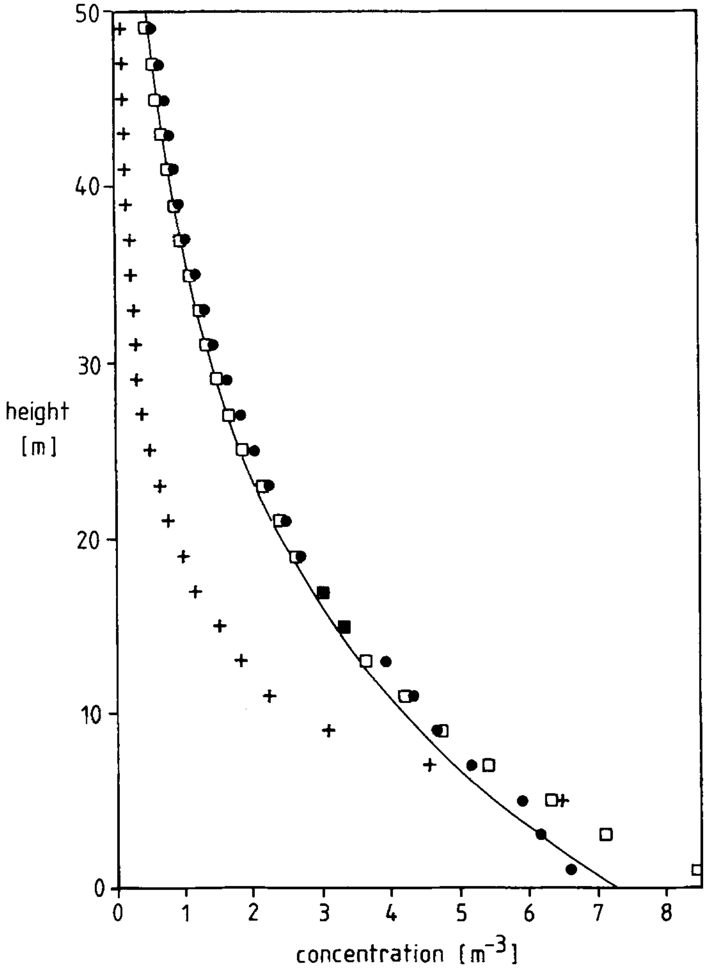

Fig. 1. The concentration profile 100 m downwind of a ground-level line source of strength $Q = 100\ \mathrm{m^{-1}\,s^{-1}}$ in turbulence with power-law profiles of windspeed and eddy diffusivity. Analytical solution (—); LR method (●); WTK″ method (□); LR with $\bar{w} = 0$ (+).

3.2. Diffusion from an elevated source in a corn canopy

A hypothetical problem of diffusion from a continuous area source of passive tracer at the top of a corn canopy was discussed by WTK. The $\bar{u}$- and σ_w-profiles used were an analytical fit to measured profiles, while τ_L was chosen so as to make the length scale a linear function of height above ground (in accordance with the observed behaviour of the length scale formed from σ_w and the Eulerian timescale of w in the same measurements).

Figure 2 shows that neither the WTK method nor the LR method gives a physically reasonable prediction for this system, in which $l(d\sigma_w/dz)$ changes rapidly with height and is not everywhere small compared with σ_w. On the other hand WTK″ gives a reasonable concentration profile – a small concentration gradient beneath the source where the vertical flux density is constrained to be small by the long fetch and the reflecting barrier at ground.

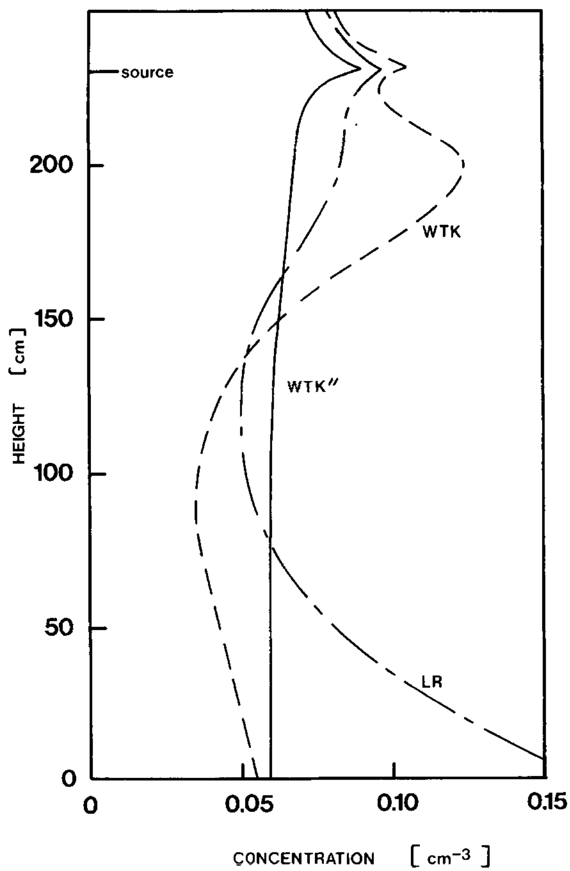

Fig. 2. The concentration profile 320 m downwind from the leading edge of an elevated area source of strength $Q = 1\ \mathrm{cm}^{-2}\,\mathrm{s}^{-1}$ in a corn canopy. See WTK for details of the turbulence. Below the source, the vertical flux and the concentration gradient may be expected to be small because the flux must vanish at the ground. Thus only the WTK″ profile seems physically reasonable.

The LR model assumes that $\mathrm{d}\sigma_w^2/\mathrm{d}z$ is constant over the duration of each distance step (which is strictly satisfied only in a system such as that of Section 3.1 having σ_w^2 a linear function of z). Modification to include a first-order correction for the height-dependence of $\mathrm{d}\sigma_w^2/\mathrm{d}z$ gave very little improvement in the LR prediction.

4. Implications for Earlier Work

Wilson (1982) has given tables of dimensionless concentration for ground-level line and area sources in the atmospheric surface layer which were calculated using the WTK method. Because the WTK method was 'calibrated' by a comparison with experimental data, these tables remain valid. However the formula given by Wilson *et al.* (1981c) for the Lagrangian length scale under unstable statification may not be the best choice for use with the LR method.

5. Conclusion

The apparent contradiction between the WTK and LR methods has been resolved. The factor of 2 difference in vertical velocity offset employed depends upon whether the Markov chain is formulated in terms of w/σ_w (WTK) or w (LR). In systems where $l(\mathrm{d}\sigma_w/\mathrm{d}z)$ changes slowly with height, WTK and LR (and WTK$'$, WTK$''$) will give similar if not identical predictions.

However, when $l(\mathrm{d}\sigma_w/\mathrm{d}z)$ changes rapidly with height, the methods are not equivalent. In the particular (and rather extreme) case examined (for which no independent solution is available), neither WTK nor LR yielded reasonable results, while a modification of WTK, here called WTK$''$, gave physically reasonable predictions. Though we can offer no proof that WTK$''$ is 'correct', it seems worthy of investigation.

References

Legg, B. J.: 1983, 'Turbulent Diffusion from an Elevated Line Source: Markov Chain Simulations of Concentraton and Flux Profiles', *Quart. J. R. Met. Soc.* **109**, 645–660.

Legg, B. J. and Raupach, M. R.: 1982, 'Markov Chain Simulation of Particle Dispersion in Inhomogeneous Flows: The Mean Drift Velocity Induced by a Gradient in Eulerian Velocity Variance', *Boundary-Layer Meteorol.* **24**, 3–13.

Pasquill, F.: 1974, *Atmospheric Diffusion*, 2nd edition, J. Wiley and Sons, New York, 429 pp.

Reid, J. D.: 1979, 'Markov Chain Simulations of Vertical Dispersion in the Neutral Surface Layer for Surface and Elevated Releases', *Boundary-Layer Meteorol.* **16**, 3–22.

Taylor, G. I.: 1921, 'Diffusion by Continuous Movements', *Proc. Lond. Math. Soc. Ser. 2* **20**, 196–212.

Wilson, J. D., Thurtell, G. W., and Kidd, G. E.: 1981a, 'Numerical Simulation of Particle Trajectories in Inhomogeneous Turbulence, I: Systems with Constant Turbulent Velocity Scale', *Boundary-Layer Meteorol.* **21**, 295–313.

Wilson, J. D., Thurtell, G. W., and Kidd, G. E.: 1981b, 'Numerical Simulation of Particle Trajectories in Inhomogeneous Turbulence, II: Systems with Variable Turbulent Velocity Scale', *Boundary-Layer Meteorol.* **21**, 423–441.

Wilson, J. D., Thurtell, G. W., and Kidd, G. E.: 1981c, 'Numerical Simulation of Particle Trajectories in Inhomogeneous Turbulence, III: Comparison of Predictions with Experimental Data for the Atmospheric Surface Layer', *Boundary-Layer Meteorol.* **21**, 443–463.

Wilson, J. D.: 1982, 'Turbulent Dispersion in the Atmospheric Surface Layer', *Boundary-Layer Meteorol.* **22**, 399–420.