RESTRICTION ON THE TIMESTEP TO BE USED IN STOCHASTIC LAGRANGIAN MODELS OF TURBULENT DISPERSION

(Research Note)

J. D. WILSON and Y. ZHUANG,

Meteorology Division, Geography Department, University of Alberta, Edmonton, Alberta T6G 2H4

(Received in final form 17 April, 1989)

Abstract. By considering two analytical solutions of G. I. Taylor (1921) for dispersion in homogeneous turbulence, we derive a quantitative upper limit for the timestep dt to be used in the stochastic Lagrangian model; a more severe upper limit will probably exist in inhomogeneous turbulence. For practical purposes, there is no lower limit to the timestep.

1. Introduction

When undertaking a discrete time simulation of turbulent dispersion using the Lagrangian stochastic (trajectory-simulation) approach, it is necessary to choose an appropriate timestep. As a guiding principle, one should choose a timestep which is much smaller than the smallest of all significant timescales in the physical system to be simulated. This leaves open the question as to what timescales must be considered significant, and in general this decision rests with the knowledge of the scientist.

The simplest case is that of the dispersion of marked fluid elements in homogeneous and stationary turbulence, for which we have available two exact solutions due to Taylor (1921) – a continuous-time solution, and also an analytical solution for the outcome of discrete-time simulations of the continuous system. In this paper, we shall discuss what limitations exist (in principle and in practice) on the choice of the timestep for simulation of dispersion in homogeneous turbulence by making use of Taylor's solutions. Restrictions which are at least as severe must arise for more general systems in which the existence of inhomogeneity may impose further criteria. To our surprise, we have found that errors arising from the choice of what hitherto seemed a reasonably small timestep, $dt = 0.2\,T_L$, where T_L is the Lagrangian integral timescale, may amount to 5% (error in the calculated plume width) at times greater than T_L.

2. Analytical Solutions and a Discrete-Time Model

Consider the release at $(z, t) = (0, 0)$ of a marked fluid element into homogeneous turbulence specified by vertical velocity variance $\overline{w^2}$, and a Lagrangian auto-

Boundary-Layer Meteorology **49**: 309–316, 1989.

correlation function $R_L(\xi)$ having an integral timescale $T_L = \int_0^\infty R_L(\xi)\,d\xi$. Taylor (1921) showed that the ensemble-averaged spread of the marked fluid elements at time t is given by

$$\overline{z^2}(t) = 2\overline{w^2}\int_0^t (t-\xi)R_L(\xi)\,d\xi\,, \tag{1}$$

It is straightforward to show that when $t \gg T_L$, the form of the autocorrelation is not relevant and that the spread depends only on $\overline{w^2}$ and T_L.

A very useful transformation of Equation (1) may be made by noting that the autocorrelation function and the Lagrangian velocity spectrum $S_w(f)$ are a Fourier Transform pair,

$$S_w(f) = 4w^2\int_0^\infty R_L(\xi)\cos(2\pi f\xi)\,d\xi\,, \tag{2a}$$

$$R_L(\xi) = \int_0^\infty (S_w(f)/\overline{w^2})\cos(2\pi f\xi)\,df\,, \tag{2b}$$

and in consequence (Pasquill and Smith, 1983), one may write

$$\overline{z^2}(t) = t^2\int_0^\infty S_w(f)\frac{\sin^2\pi ft}{(\pi ft)^2}\,df\,. \tag{3}$$

This equation shows that the 'lowest' frequencies in the velocity spectrum are most effective in bringing about plume dispersion, and that as t increases, the effectiveness rests with ever lower frequencies. We shall make use of this equation in Section 4.

We shall now outline a standard discrete-time model of this problem. The position of the fluid element at time $t = n\,dt$ is

$$z(n\,dt) = \sum_{k=1}^{n}\Delta z_k\,, \tag{4}$$

where $\Delta z_k = w_k\,dt$. We shall assume the velocity time series is to be generated by the Markov chain

$$w_{k+1} = \alpha w_k + \beta r_{k+1}\,, \tag{5}$$

where α is the correlation between consecutive discrete velocity samples and the term βr_{k+1} is a random change, the product of a normalising factor β (defined below) and r_{k+1}, a random number drawn from a Gaussian distribution having zero mean and unit variance. (By the Central Limit Theorem, equally acceptable

results follow with r_i randomly chosen as $+1$ or -1, provided that the time t of interest greatly exceeds $\mathrm{d}t$.)

By manipulating Equation (5) it is easy to show that, to attain the desired velocity variance, one requires $\beta = \sqrt{1-\alpha^2}\,\sigma_w$, where σ_w is the velocity standard deviation. Similarly, the correlation between velocities separated by an arbitrary number of timesteps can be shown to be $R(k\,\mathrm{d}t) = [R(\mathrm{d}t)]^k = \alpha^k$ so that, to ensure $\sum_{k=1}^{\infty} R(k\,\mathrm{d}t)\,\mathrm{d}t = T_L$, one requires $\alpha = 1 - \mathrm{d}t/T_L$.

There are several ways to justify the use of Equation (5). Firstly, it is the simplest numerical procedure by which one may obtain a velocity series having the correct velocity variance and autocorrelation timescale (which Taylor's solution proves are the only factors governing the rate of spread in homogeneous turbulence for $t \gg T_L$). Secondly, theoretical arguments have been given (Lin, 1960; van Dop *et al.*, 1985; Haworth and Pope, 1986) that this model is implied by the Navier–Stokes equations for the case of very high Reynold's number turbulence. And thirdly, one may appeal to the agreement of observations with such a model (Hanna, 1979).

To carry out a discrete simulation of the dispersion problem, one must specify the physical scales, initialise the Markov chain ($w_1 = \sigma_w r_1$), and select a value for the timestep: say

$$\mathrm{d}t = \mu T_L \qquad (\mu < 1)\,. \tag{6}$$

The outcome of a discrete simulation of spread in homogeneous turbulence may be anticipated, because it is easy to calculate the ensemble mean value of $z^2(n\,\mathrm{d}t) = (\mathrm{d}z_1 + \mathrm{d}z_2 + \cdots + \mathrm{d}z_n)^2$. The result was given by Taylor (1921; the unnumbered equation preceding his Equation (2)). However we believe Taylor's formula is wrong; for example, setting $n = 1$ in that equation, one obtains for the mean square displacement after only one step, a result which is held to depend upon α, the correlation of that step with the (as yet untaken) second step. We believe that the formula should read

$$\overline{z^2}(n\,\mathrm{d}t) = \overline{w^2}\,\mathrm{d}t^2 \left[n + 2\alpha^n \frac{\alpha^{-1} + \left(\dfrac{n-1}{\alpha} - n\right)\alpha^{-n}}{(1-\alpha^{-1})^2} \right] \tag{7a}$$

$$= \overline{w^2}\,\mathrm{d}t^2 \left[n + \frac{2(n-1)\alpha}{1-\alpha} - \frac{2\alpha^2(1-\alpha^{n-1})}{(1-\alpha)^2} \right]. \tag{7b}$$

Our result (7b) differs from Taylor's only in that, where we have $(n-1)$ appearing in the second and third terms on the right-hand side, Taylor has n. If, for example, we set $\alpha = 0.9$, the normalised spread $\overline{z^2}/(\overline{w^2}\,\mathrm{d}t^2)$ after $n = 2$ steps is predicted to be 3.80 (our equation) as opposed to 7.22 (Taylor's equation). Numerical simulation confirms our result.

We are now in a position to discuss various limitations on the choice of the timestep.

3. Lower Limit to the Timestep

No matter how small the timestep $\mathrm{d}t$, the Markov chain will generate a velocity series which has the Markovian property, i.e.,

$$p(w_{k+1}|\, w_k,\, w_{k-1},\, \ldots,\, w_1) = p(w_{k+1}|\, w_k)\,. \tag{8}$$

The acceleration of a real fluid element is correlated over a time interval of the order of T_λ, the acceleration timescale, which is of the order of the Kolmogorov timescale. Therefore a real velocity series at increments $\mathrm{d}t < T_\lambda$ cannot be Markovian and Equation (5) is in principle correct only under the restriction that $\mathrm{d}t \gg T_\lambda$ (Legg and Raupach, 1982). One could not use the Markov chain with a very small timestep $\mathrm{d}t \ll T_\lambda$ and achieve a realistic calculation of the spread at very short travel times $t \sim T_\lambda$. In practice, however, one is not interested in such a short travel time, and the choice of a timestep smaller than T_λ should have no adverse consequences. (In a similar way, the use of a random walk with *independent* increments is physically realistic only if the timestep, and thus the travel time, exceed the velocity correlation timescale – the use of a timestep $\mathrm{d}t < T_L$ would in such a case have no deleterious effect on the prediction of the spread at $t \gg T_L$ but would not give correct results at small t no matter how small the timestep.) Thus we believe that for practical purposes, there is no lower limit to the choice of the timestep.

In order to give an intuitive understanding of the fact that unlimited decreases in the timestep (higher resolution trajectories) do not result in any alteration in the rate of dispersion, it is useful to examine the relationship between the generated (simulated) velocity spectrum and the timestep employed. In the appendix, it is shown that if a velocity series is generated using the Markov chain Equation (5), the power spectrum of that velocity series is

$$S_w(f) = \frac{\overline{w^2}}{f_N}\,\frac{1-\alpha^2}{1+\alpha^2-2\alpha\cos(2\pi f\,\mathrm{d}t)}\,, \tag{9}$$

for $0 \leqslant f \leqslant f_N$ where $f_N = 1/(2\,\mathrm{d}t)$ is the Nyquist frequency. It is easy to show that

$$\int_0^\infty S_w(f)\,\mathrm{d}f = \overline{w^2}\,, \tag{10}$$

and

$$\frac{S_w(0)}{\overline{w^2}} = 4\,T_L(1-\mu/2) \xrightarrow[0]{\mu} 4\,T_L\,. \tag{11}$$

It follows from Equation (11) that, provided $\mu < 0.1$, the spectral density at the origin is within 5% of its limiting value as $\mathrm{d}t \to 0$.

Power spectra corresponding to simulation of trajectories with differing values of the timestep are not identical because a reduction in $\mathrm{d}t$ results in a spectrum

which extends to a higher frequency, because the power spectrum for the random Gaussian variable r is $S_r(f) = 1/f_N$ and has more power at low frequency. We know from Taylor's Equation (1) that the spread (at given t) should not change as $dt \to 0$, yet the velocity spectrum which is effective in causing the (simulated) spread *does* change as $dt \to 0$. The insensitivity of the spread to the alterations in the Lagrangian spectrum as dt varies is a consequence of the fact that, as indicated by Equation (3), the low frequency end of the spectrum is most effective in contributing to the spread – and at the low frequency end, there is little variation in the spectrum as dt takes on different values less than about $0.1\,T_L$.

4. Upper Limit to the Timestep

It is certain that one must ensure $dt < T_L$: otherwise the *effective* correlation time will default to dt, because the velocity cannot persist for a time which is less than the timestep. However one would like to know just how much smaller than T_L the timestep must be, because the generation of trajectories requires much computer time and one is often tempted to increase the timestep. Most authors have used $dt = 0.1\,T_L$ or $dt = 0.2\,T_L$.

The question is easily resolved by comparing Taylor's analytical solution for the discrete process (which explicitly involves the timestep) with his time-continuous solution (which does not involve any timestep). We have evaluated the continuous time solution for the case of an exponential autocorrelation

$$R(\xi) = \exp(-\xi/T_L). \tag{12}$$

Calculations were performed for a system having $T_L = 1$, $\sigma_w = 1$. Table I tabulates both analytical solutions for the plume width $\sigma_z(t) = \overline{z^2}^{1/2}$ and the percentage error in the discrete solution relative to the continuous solution as a function of the ratio dt/T_L for a range of travel times t. It is apparent that with a timestep as large as $0.25\,T_L$, an error in the spread amounting to more than 5% occurs for relatively long (far field) travel times, while a doubling to $0.5\,T_L$ yields an error exceeding 10%. The implication is that before attempting to incorporate complexities such as streamwise velocity fluctuation, velocity cross-correlation, etc., in order to attain very close agreement (error < 5%) with experiment, the user of this type of model should ensure that the timestep is sufficiently small. For homogeneous turbulence, a timestep $dt = 0.1\,T_L$ is sufficiently small to hold the discretisation error in the plume width to about 2%.

These results may have been anticipated on the basis of the earlier-examined dependence of $S_w(0)$ on dt/T_L: as the timestep becomes large, the spectral density at low frequency decreases and, by Equation (3), we expect a simulation to underestimate the spread.

TABLE I

Discrete and continuous solutions (σ_z^{dis} and σ_z^{cts}, respectively) for the plume width σ_z as a function of travel time t/T_L, showing the percentage error in the discrete solution for each of several values of the timestep $\Delta t/T_L$.

	$t/T_L = 0.5$ ($\sigma_z^{cts} = 0.462$)		$t/T_L = 1.0$ ($\sigma_z^{cts} = 0.858$)	
$\Delta t/T_L$	σ_z^{dis}	Error (%)	σ_z^{dis}	Error (%)
0.01	0.461	−0.04	0.857	−0.07
0.05	0.461	−0.11	0.855	−0.32
0.1	0.461	−0.04	0.853	−0.56
0.25	0.468	1.3	0.851	−0.76
0.50	0.500	8.3	0.866	0.96
	$t/T_L = 2$ ($\sigma_z^{cts} = 1.51$)		$t/T_L = 5$ ($\sigma_z^{cts} = 2.83$)	
$\Delta t/T_L$	σ_z^{dis}	Error (%)	σ_z^{dis}	Error (%)
0.01	1.51	−0.1	2.83	−0.2
0.05	1.50	−0.6	2.80	−1.0
0.1	1.49	−1.2	2.78	−1.9
0.25	1.47	−2.7	2.69	−4.9
0.50	1.44	−4.7	2.55	−9.9
	$t/T_L = 10$ ($\sigma_z^{cts} = 4.24$)		$t/T_L = 50$ ($\sigma_z^{cts} = 9.90$)	
$\Delta t/T_L$	σ_z^{dis}	Error (%)	σ_z^{dis}	Error (%)
0.01	4.23	−0.2	9.87	−0.3
0.05	4.20	−1.1	9.78	−1.2
0.1	4.15	−2.3	9.65	−2.5
0.25	4.00	−5.7	9.27	−6.3
0.50	3.74	−11.8	8.60	−13.1

5. Conclusion

There is no lower limit to the choice of a timestep for the Lagrangian stochastic dispersion model. However, an upper limit of $dt = 0.1\,T_L$ is suggested if one wishes to be sure that time discretisation causes an error of less than about 2%. If an error of the order of 15% is acceptable (still a small error compared to likely errors stemming from the use of cruder types of dispersion model), the timestep may be as large as $0.5\,T_L$. These results can readily be extended to the case of a longer travel time than given here.

No rigorous extension to inhomogeneous turbulence is possible, but the limitation is unlikely to be less severe. To give an example, in the neutral

atmospheric surface layer, the Lagrangian timescale varies with height as $T_L = az/\sigma_w$, with $a \sim 0.5$ (Sawford, 1985; there is uncertainty surrounding the exact value of a). Defining a length scale $L = \sigma_w T_L$, we obtain an 'inhomogeneity timescale' $T^* = L\,\mathrm{d}T_L/\mathrm{d}z = aT_L$. But we began by stating the principle that the timestep should be much smaller than the smallest of the significant timescales. Therefore, since $T^* < T_L$, it is possible that the timestep must be restricted more severely in this case than in the homogeneous case.

Appendix: The Velocity Spectrum Generated by the Markov Chain

We assume an infinite record length, sampled at intervals $\mathrm{d}t$. In such a circumstance we may define a Fourier Transform pair as (Otnes and Enochson, 1972; "Type II" transform):

$$X(f) = \mathrm{d}t \sum_{r=-\infty}^{\infty} x_r \exp[-j2\pi fr\,\mathrm{d}t],$$

$$x(t) = \int_{-1/2\,\mathrm{d}t}^{1/2\,\mathrm{d}t} X(f) \exp[j2\pi ft]\,\mathrm{d}f.$$

With this definition, Fourier transformation of Equation (5) yields the result that the Fourier Transform of $w(t)$ is

$$W(f) = G(f)\frac{\beta}{\exp[j2\pi f\,\mathrm{d}t] - \alpha},$$

where $G(f)$ is the Fourier Transform of the time series of the random Gaussian variable. Multiplying both sides by the complex conjugate and noting that the spectrum of the random noise is white out to the Nyquist frequency, $S_r(f) = 1/f_N$, we obtain Equation (9).

References

Hanna, S. R.: 1979, 'Some Statistics of Lagrangian and Eulerian Wind Fluctuations', *J. Appl. Meteorol.* **18**, 518–525.

Haworth, D. C. and Pope, S. B.: 1986, 'A Generalised Langevin Model for Turbulent Flows', *Phys. Fluids* **29**, 387–405.

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

Lin, C. C.: 1960, 'On a Theory of Diffusion by Continuous Movements', *Proc. Nat. Acad. Sci.* **46**, 566.

Otnes, R. K. and Enochson, L.: 1972, *Digital Time Series Analysis*, J. Wiley & Sons, Inc.

Pasquill, F. and Smith, F. B.: 1983, *Atmospheric Diffusion*, 3rd Edition, J. Wiley & Sons, Inc.

Sawford, B. L.: 1985, 'Lagrangian Statistical Simulation of Concentration Mean and Fluctuation Fields', *J. Clim. Appl. Meteorol.* **24**, 1152–1166.

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

van Dop, H., Nieuwstadt, F. T. M., and Hunt, J. C. R.: 1985, 'Random Walk Models for Particle Displacements in Inhomogeneous Unsteady Turbulent Flows', *Phys. Fluids* **28**, 1639–1653.