Qualitative Modelling of Turbulent Diffusion

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Abstract A qualitative model of turbulent diffusion introduced by Zimmerman & Chatwin (1995, *Environmetrics*, **6**, 665–675), henceforth referred to as ZC, is considered. In this model the diffusion equation is solved in a one-dimensional finite region, with zero concentration gradient imposed at the ends of the region. This is equivalent to an unbounded periodic problem. Randomness is introduced into the model (to simulate the effect of random turbulent advection) by taking the sampling position to be random. ZC took as initial condition a symmetrically positioned rectangular "pulse". The results gave a a bimodal probability density function (pdf), with peaks at the minimum and maximum concentrations, and also gave a collapse of the concentration kurtosis against the concentration skewness for narrow initial pulses. Asymptotic analysis shows that the former result must hold at large time for any symmetric initial condition. We examine a generalisation of the ZC model to asymmetric initial conditions. These cases can be transformed to problems with symmetric initial conditions, so the large time pdf must be bimodal. For narrow rectangular pulse initial conditions the kurtosis-skewness collapse is also obtained. In nearly all of these cases the large time behaviour is of the same form as for a symmetrically positioned pulse of the same width, but with a time scale 4 times greater. It is suggested that to obtain results relevant to turbulent diffusion the most significant improvement can be made by incorporating a more realistic velocity field into the model. However, it is also proposed that more representative results might be obtained by averaging the results for the asymmetrically positioned pulse over a suitable ensemble of pulse displacements from the central position.

1. INTRODUCTION

Turbulent diffusion is a process of considerable interest in both environmental (e.g. dispersion of pollutants in the atmosphere) and engineering (e.g. in combustion processes) contexts. In the relatively simple case of diffusion of a conserved (i.e. non-reacting) scalar $\Gamma(\mathbf{x},t)$ (to be referred to as the concentration), the governing equations are

$$\frac{\partial \Gamma}{\partial t} + \mathbf{u}\cdot\nabla\Gamma = \kappa\nabla^2\Gamma, \qquad (1)$$

where $\mathbf{u}(\mathbf{x},t)$ is the turbulent velocity and κ is the molecular diffusivity, together with the Navier-Stokes and continuity equations for $\mathbf{u}$. The randomness of $\mathbf{u}$ and, hence, of Γ, together with the nonlinearity of the equations, means that a closed set of equations cannot be obtained even for the mean velocity and mean concentration. For this reason modelling of turbulent diffusion usually proceeds by approximating the equations so that a closed set is obtained. In all such models accurate representation of all relevant physical processes is sacrificed in order to be able to obtain a solution.

The focus in this paper is on a particular qualitative model of turbulent diffusion which was first presented by Zimmerman & Chatwin [1995b] (henceforth referred to as ZC), and was developed further in Chatwin & Zimmerman [1998] and Zimmerman [1996]. In the first version of this model the only physical processes included were molecular diffusion and random advection (effectively on large scales, with no spatial variation), and only 1 space dimension was retained. This model was able to reproduce certain observed features, for example the collapse onto an approximately quadratic curve of the graph of kurtosis against skewness (first noted by Mole & Clarke [1995], and subsequently by, for example, Zimmerman & Chatwin [1995a], Lewis & Chatwin [1995], Heagy & Sullivan [1996], Li & Bilger [1996] and Chatwin & Robinson [1997]).

In the original ZC model (1) is replaced by

$$\frac{\partial \Gamma}{\partial t} = \kappa\frac{\partial^2 \Gamma}{\partial x^2}, \qquad (2)$$

and is solved on the 1D domain $-l \le x \le l$, together with the boundary condition

$$\frac{\partial \Gamma}{\partial x} = 0 \qquad \text{at } x = \pm l, \qquad (3)$$

and a prescribed initial condition $\Gamma(x,0)$. (3) implies that the solution will be equivalent to a periodic solution in $-\infty < x < \infty$ with period $2l$. Randomness is introduced into the model by assuming that the measurement position is random, with a uniform distribution on $[-l, l]$. This is equivalent to fixing the measurement position and allowing random (but rigid) movement of the diffusing scalar.

Introducing non-dimensional variables

$$X = \frac{x}{l}, \quad T = \frac{\kappa t}{l^2}, \quad C(X,T) = \frac{\Gamma(x,t)}{\Gamma_0},$$

where Γ_0 is a representative scale for $\Gamma(x,0)$, gives

$$\frac{\partial C}{\partial T} = \frac{\partial^2 C}{\partial X^2} \qquad -1 \le X \le 1 \qquad (4)$$

$$\frac{\partial C}{\partial X} = 0 \qquad \text{at } X = \pm 1 \qquad (5)$$

$$C(X,0) = g(X) \qquad -1 \le X \le 1, \qquad (6)$$

for some function g. Concentration moments are then given by

$$\mu = E\{C\} = \frac{1}{2}\int_{-1}^{1} C(X,T)dX = \frac{1}{2}\int_{-1}^{1} g(X)dX,$$

which is a constant, and

$$\mu_n(T) = E\{(C-\mu)^n\} = \frac{1}{2}\int_{-1}^{1} (C(X,T)-\mu)^n \, dX. \qquad (7)$$

(Here $E\{\cdot\}$ denotes the mean, or expected value.) The variance σ^2, skewness S and kurtosis K are defined by

$$\sigma^2 = \mu_2, \quad S = \frac{\mu_3}{\sigma^3}, \quad K = \frac{\mu_4}{\sigma^4}. \qquad (8)$$

2. SYMMETRIC INITIAL CONDITION

Suppose the initial condition $g(X)$ is symmetric about $X = 0$. Then the solution to (4)–(6) can be written as

$$C(X,T) = \mu + \sum_{n=1}^{\infty} A_n \cos(n\pi X) e^{-n^2\pi^2 T}, \quad (9)$$

where

$$A_n = 2\int_0^1 g(X)\cos(n\pi X)dX.$$

It then follows from (7) and (8) that

$$\sigma^2 = \frac{1}{2}\sum_{n=1}^{\infty} A_n^2 e^{-2n^2\pi^2 T} \qquad (10)$$

$$\mu_3 = \frac{3}{4}\sum_{k,m=1}^{\infty} A_k A_m A_{k+m} \times e^{-2(k^2+m^2+km)\pi^2 T} \qquad (11)$$

$$\mu_4 = \frac{1}{2}\sum_{k,m,n=1}^{\infty} A_k A_m A_n A_{k+m+n} \times e^{-2(k^2+m^2+n^2+km+kn+mn)\pi^2 T} + \frac{3}{8}\sum_{\substack{k,m,n=1\\ k+m>n}}^{\infty} A_k A_m A_n A_{k+m-n} \times e^{-2(k^2+m^2+n^2+km-kn-mn)\pi^2 T}. \qquad (12)$$

By retaining only the terms up to $n = 2$ in (9) the large time asymptotic solution of ZC can be obtained:

$$\sigma^2 \approx \frac{1}{2}A_1^2 e^{-2\pi^2 T}\left[1 + \left(\frac{A_2}{A_1}\right)^2 e^{-6\pi^2 T}\right] \quad (13)$$

$$S^2 \approx \frac{9}{2}\left(\frac{A_2}{A_1}\right)^2 e^{-6\pi^2 T} \times \left[1 - 3\left(\frac{A_2}{A_1}\right)^2 e^{-6\pi^2 T}\right] \qquad (14)$$

$$K \approx \frac{3}{2}\left[1 + 2\left(\frac{A_2}{A_1}\right)^2 e^{-6\pi^2 T}\right] \qquad (15)$$

$$K \approx \frac{3}{2} + \frac{2}{3}S^2. \qquad (16)$$

ZC calculated numerical solutions from the initial condition

$$g(X) = \begin{cases} 1 & |X| \le \gamma \\ 0 & \text{otherwise,} \end{cases} \qquad (17)$$

where $0 < \gamma < 1$. In this case $\mu = \gamma$ and

$$A_n = \frac{2}{n\pi}\sin(n\pi\gamma). \qquad (18)$$

The numerical results for various values of γ were in agreement with the asymptotic results (13)–(16), and also with some small time asymptotic results derived in ZC.

The numerical results of ZC showed that the probability density function (pdf) of concentration was bimodal, with peaks at the minimum and maximum concentrations, and that at large time these concentration bounds converged towards the mean concentration μ. Chatwin & Zimmerman [1998] derived this result analytically for small and large time. In fact, this large time behaviour is inevitable in this model for any symmetric $g(X)$, since eventually $C-\mu$ will be dominated by the leading term for which A_n does not vanish, A_m say. Peaks occur in the pdf at the values of C for which $\partial C/\partial X = 0$, i.e. at

$$C = \gamma \pm A_m e^{-m^2\pi^2 T}.$$

3. ASYMMETRIC INITIAL CONDITION

3.1 Analytical Results

For any initial condition $g(X)$ the equivalent periodic problem implied by the boundary condition (5) can be transformed into a problem with symmetric initial condition by defining

$$X' = \frac{1}{2}(X-1), \qquad T' = \frac{1}{4}T. \qquad (19)$$

(4) and (5) then apply with T and X replaced by T' and X', and with initial condition

$$C(X',0) = \begin{cases} g(1+2X') & -1 \le X' \le 0 \\ g(1-2X') & 0 \le X' \le 1. \end{cases} \qquad (20)$$

Thus the solution (9), and the moments (10)–(12), also apply, with T and X replaced by T' and X', and A_n calculated from $C(X',0)$ rather than from $g(X)$. The implication is that, provided $A_1 \neq 0$ and $A_2 \neq 0$, the asymptotic form of the moments (as given by (13)–(16)) and of the pdf is the same for symmetric and asymmetric initial conditions, but that the time scale is 4 times greater in the asymmetric case. (Of course the moments will also differ because of the different values of A_1 and A_2.)

3.2 Numerical Results

We calculated numerical solutions of (4)–(6) (by a finite difference scheme, rather than by truncating (9)), using asymmetric initial conditions analogous to those of ZC, i.e.

$$g(X) = \begin{cases} 1 & |X - X_0| \le \gamma \\ 0 & \text{otherwise.} \end{cases} \qquad (21)$$

Here we consider only $\gamma < 1/2$, since in turbulent diffusion, except very close to the source, we expect small values of γ to be relevant. Without loss of generality $0 \le X_0 \le 1-\gamma$. $X_0 = 0$ gives the ZC initial conditions. Under (19) the $X_0 = 1-\gamma$ case transforms exactly to the ZC case, and so has exactly the same solution, but with a time scale 4 times greater. For $0 < X_0 < 1-\gamma$, from the previous subsection, we expect, provided that $A_1 \neq 0$ and $A_2 \neq 0$, that at large time the moments will be approximately the same as those for $X_0 = 1-\gamma$ (with the precise differences depending on the values of the A_n). The equivalent periodic problem has initial rectangular "pulses" with two separation distances $2(1 \pm X_0)$. At large time the pulses separated by $2(1-X_0)$ effectively merge and the result is close to that obtained from one symmetrically positioned initial pulse of twice the width, which is equivalent to the $X_0 = 1-\gamma$ case. The larger X_0, and thus the smaller $2(1-X_0)$, the earlier we expect the pulses to merge, and so the earlier we would expect there to be a transition from behaving like the $X_0 = 0$ case to behaving like the $X_0 = 1-\gamma$ case. The exception to this behaviour, as described below, is $X_0 = 1/2$, for which $A_2 = 0$. For X_0 close to $1/2$, A_2 will be very small, so that although the ultimate asymptotic form will be different from that of $X_0 = 1/2$, it will take a long time for that asymptotic form to be reached.

At small times, before diffusion has carried a significant amount of scalar to the boundary $X = 1$, we expect the moments to be approximately the same as for $X_0 = 0$. Thus we expect the small time approximation of ZC will be valid, but that it will break down at earlier times for larger X_0. This is confirmed by the numerical solutions.

Calculating A_n using (20) and (21) gives

$$A_n = \frac{4}{n\pi}\sin\left(\frac{1}{2}n\pi\gamma\right)\cos\left[\frac{1}{2}n\pi(1-X_0)\right]$$

for $X_0 \neq 0$. Thus (13)–(16) apply, except in the case $X_0 = 1/2$ when $A_2 = 0$ and (10)-(12) lead to

$$\sigma^2 \approx \frac{1}{2} A_1^2 e^{-2\pi^2 T'} \left[1 + \left(\frac{A_3}{A_1} \right)^2 e^{-16\pi^2 T'} \right]$$

$$S^2 \approx 18 \left(\frac{A_3 A_4}{A_1^2} \right)^2 e^{-46\pi^2 T'} \times \left[1 + \left\{ 2\frac{A_5}{A_3} - 3 \left(\frac{A_3}{A_1} \right)^2 \right\} e^{-16\pi^2 T'} \right]$$

$$K \approx \frac{3}{2} \left(1 + \frac{4A_3}{3A_1} e^{-8\pi^2 T'} \right)$$

$$K \approx \frac{3}{2} + \frac{2A_3^{15/23}}{18^{4/23} A_1^{7/23} A_4^{8/23}} S^{8/23}.$$

So for $X_0 = 1/2$ the large time asymptotic behaviour is different from that in the symmetric case. The skewness decays more quickly than in the symmetric case $X_0 = 0$, while the kurtosis decays more slowly than in the symmetric case.

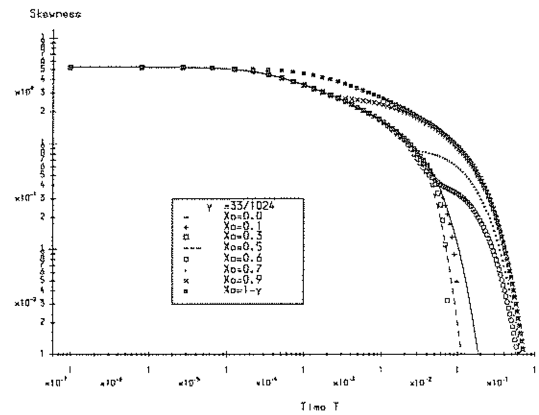

Figure 1: Skewness S against time T for $\gamma = 33/1024$.

The dependence of the results on γ is similar to that found in ZC, so here we concentrate on the effect of varying X_0. Figure 1 shows the time variation of S for $\gamma = 33/1024$ and for various values of X_0. As expected, at small times the skewness is independent of X_0. For large X_0 the behaviour is as described above, with a transition from $X_0 = 0$ to $X_0 = 1-\gamma$ behaviour, with an earlier transition for larger X_0. For $X_0 = 0.5$ the skewness decays faster than for $X_0 = 0$, as expected, while for $X_0 = 0.1, 0.3$ the skewness is similar to that for $X_0 = 0.5$. In the latter cases we expect that eventually there will be a transition to $X_0 = 1 - \gamma$ behaviour.

As shown in Figure 2, similar behaviour is observed for the kurtosis, but with some additional

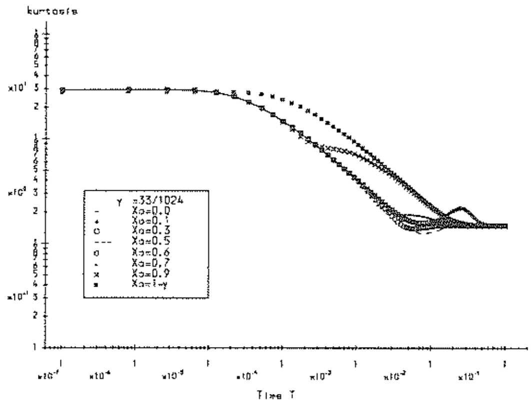

Figure 2: Kurtosis K against time T for $\gamma = 33/1024$.

variation in the behaviour as the asymptotic limit of 1.5 is approached, with the kurtosis dipping below 1.5 in some cases. (15) shows that the ultimate approach to 1.5 is from above, except for $X_0 = 0.5$ when the approach is from below.

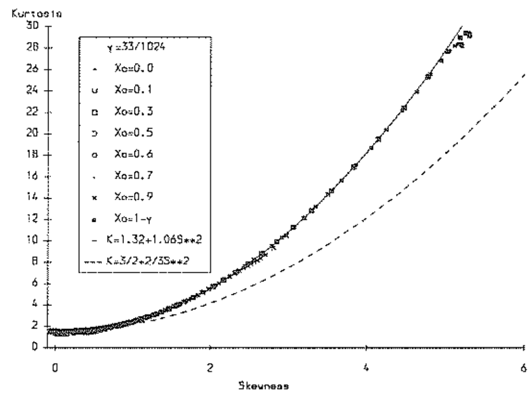

Figure 3: Kurtosis against skewness for $\gamma = 33/1024$. The small time (solid line) and large time (dashed line, equation (16)) asymptotic approximations are also shown.

Figure 3 shows the kurtosis plotted against the skewness for $\gamma = 33/1024$ and various values of X_0. The collapse onto something close to a single curve is striking. The greatest scatter in the results appears to be at large time when S and K are small.

Figures 4–7 show the pdf (estimated from a histogram derived from the numerical solution for $C(X,T)$ at the X gridpoints) at four times, for $\gamma = 33/1024$ and $X_0 = 0.5$. At $T = 0.01$ the

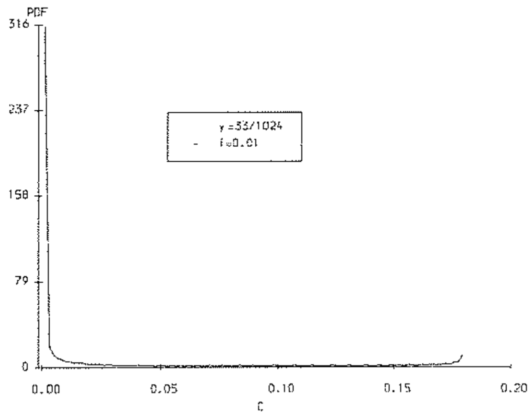

Figure 4: Pdf for $\gamma = 33/1024$ and $X_0 = 0.5$ at $T = 0.01$.

pdf is bimodal as for the symmetric case of ZC (although the peak at the maximum concentration is not very well resolved). Once a significant amount of material has diffused to the boundary at $X = 1$ the concentration starts building up there, so that a third peak in the pdf emerges at the minimum concentration and moves progressively to larger concentrations until it merges with the upper peak, and the asymptotic bimodal development sets in.

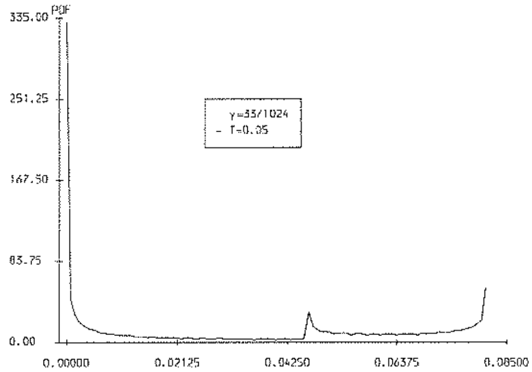

Figure 5: Pdf for $\gamma = 33/1024$ and $X_0 = 0.5$ at $T = 0.05$.

4. DISCUSSION

As a model of turbulent diffusion, the model of ZC is unrealistic in several ways, including the following: the model has only one space dimension; in effect spatial variation of the advecting velocity is ignored; and the concentration structure does not reflect the complexity of that in turbulent diffusion. The periodicity in the model forces the large time pdf to be bimodal, with peaks at the smallest and largest concentrations, regardless of the initial concentration structure. While Chatwin & Zimmerman [1998] argued that there is no *a priori* reason to reject such bimodal pdfs, it seems unsatisfactory that the bimodality at later times in the ZC model follows directly from the artificial periodic structure of the model.

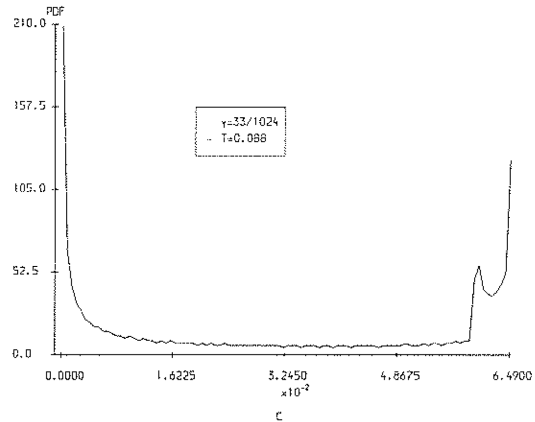

Figure 6: Pdf for $\gamma = 33/1024$ and $X_0 = 0.5$ at $T = 0.088$.

Similar results hold even if the number of space dimensions is increased and, as discussed in §3.1, for more complex concentration structures. At intermediate times the results of §3.2 showed that an increase in complexity of the structure can lead to more than two peaks in the pdf, a feature for which there is no evidence in turbulent diffusion from sources of uniform concentration. Zimmerman [1996] considered an extension of the model to 3 space dimensions with advection by a spatially varying velocity field which has chaotic streamlines. The numerical results gave a large time unimodal pdf, but still gave a $K - S$ collapse. So the extension to the ZC model which seems most likely to produce results relevant to turbulent diffusion is to introduce a more realistic velocity field. The model may in any case be more useful as a limiting test case for more realistic models of turbulent diffusion.

The $K - S$ collapse seems to be a robust feature. It occurs in the original ZC model where the pdf is bimodal, in our asymmetric modification (see Figure 3), where the pdf can have more than 2 peaks, and in the model of Zimmerman [1996], where the pdf soon becomes unimodal. The existence of the collapse over such a range of pdfs raises the question of how much the collapse actually tells us about the pdf, other than that the pdf can probably be represented quite

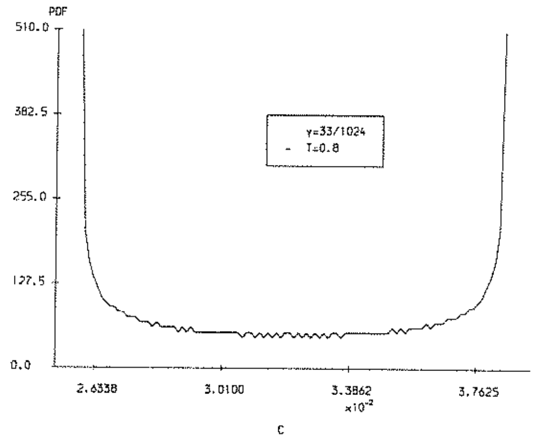

Figure 7: Pdf for $\gamma = 33/1024$ and $X_0 = 0.5$ at $T = 0.8$.

well by 3 parameters.

As noted by Chatwin & Zimmerman [1998], similar bimodal pdfs to those of the ZC model were derived by Kowe & Chatwin [1985] for a cloud of scalar diffusing in a simple random velocity field. In that case the bimodal pdfs were also used in simulating pdfs for more realistic velocity fields, in some cases leading to a unimodal pdf. A similar use could be made of the results from the model of §3.2, recognising that in turbulent diffusion there are "strands" of scalar with a range of random separations. Thus the pdf $p_A(\theta; T, X_0, \gamma)$ produced by the model of §3.2 could be averaged over X_0, using an assumed probability distribution $f(\chi)$ for X_0, to give an overall pdf $p(\theta; T, \gamma)$. Thus

$$p(\theta; T, \gamma) = \int_0^{1-\gamma} f(\chi) p_A(\theta; T, \chi, \gamma) d\chi.$$

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