ON THE MOMENTS APPROXIMATION METHOD FOR CONSTRUCTING A LAGRANGIAN STOCHASTIC MODEL

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Abstract. The exact Eulerian velocity probability density function (pdf) of a turbulent field is generally unknown, and one normally has available only partial information in the form of low order moments. We compare two alternative Lagrangian Stochastic (LS) approaches formed from this partial information, (i) the "moments approximation" approach (Kaplan and Dinar, 1993); and (ii) the well-mixed model (Thomson, 1987) that corresponds to the "maximum missing information" pdf formed from the available information. We show that the moments approximation model does not in general satisfy the well-mixed constraint, and can give an inferior prediction of dispersion.

1. Introduction

In studies of turbulent dispersion, it is usual to treat the underlying turbulent flow as "statistically known," the notion normally indicating no more than that means and variances of the turbulent velocity field are specified. This has been completely satisfactory for simple (e.g., gradient-diffusion) models of dispersion, which hinge on rudimentary flow knowledge. But modern Lagrangian stochastic (LS) "Random Flight" models, which are used to calculate an ensemble of turbulent trajectories and thus to mimic dispersion, call for and can usefully employ, a deeper statistical knowledge of the flow: and so give sharper definition to what is implied (in the context of dispersion) by calling a flow "known."

Since Thomson's (1987) provision of a selection criterion for LS models (the "well-mixed condition," Section 2), "known flow" has come to mean that the probability density function (pdf) p_a of the Eulerian velocity field is a mathematically-known function of position. The beauty of Thomson's criterion is that, given complete Eulerian information (p_a), one may derive (with reasonable assumptions) a consistent (though not necessarily unique) trajectory model. Further (rigorous) developments can only pin trajectory models to an even more complete specification of the turbulent flow (e.g., two-point, joint pdf's).

Here we focus on the fact that only for ideal flows is the velocity pdf p_a completely known. For any real flow, one has available only partial information on p_a, probably in the form of a few low-order moments. The LS model for any real flow, therefore, must be built from partial information. To overcome this

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difficulty, Kaplan and Dinar[1] (1992, 1993) introduced a "moments approximation," whereby only a finite number of moments of the Eulerian turbulent velocity is needed. The Kaplan–Dinar method relieves the derivation of a trajectory model equation of any fundamental difficulty, but a number of questions remain to be answered:

(i) Does the moments approximation model satisfy the well-mixed constraint?
(ii) How many terms in the power series for the conditional mean acceleration of a particle need to be retained, to obtain a satisfactory simulation?
(iii) How many moments are to be involved?

We shall address these questions, and we consider also an alternative approach to building an LS model from partial information on the flow (via the "maximum missing information" pdf corresponding to the given information). We confine our attention to steady-state, one-dimensional problems.

2. The Exact Model and the Approximate Model

The general form of a one-dimensional LS model for the evolution of particle state (z, w) under steady state flow conditions is (Thomson, 1987)

$$dw = a(w, z)\, dt + b(w, z)\, d\xi\,, \tag{1}$$

$$dz = w\, dt\,. \tag{2}$$

Here $a(w, z)$ is the conditional mean particle acceleration, and $b(w, z)\, d\xi$ is a random forcing, $d\xi$ being a Gaussian random number with mean zero and variance dt.

2.1. The well-mixed constraint

Corresponding to (1) and (2) is a Fokker–Planck equation which governs the evolution of the joint position-velocity pdf of dispersing particles, $p(w, z, t)$:

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial z}(wp) - \frac{\partial}{\partial w}(ap) + \frac{1}{2}\frac{\partial^2}{\partial w^2}(b^2 p)\,. \tag{3}$$

Suppose tracer particles are released at $t = 0$ such that

$$p(w, z, 0) \propto \rho(z) p_a(w, z)\,,$$

where ρ is the fluid density (henceforth assumed constant), and p_a is the Eulerian velocity pdf: then the tracer particles are "well- mixed" with respect to position and velocity. It is natural to expect that they remain well mixed, so that for all t,

[1] The Kaplan–Dinar model is comprehensive in that it is intended to be applicable to the calculation of multi-particle trajectories (with correct relative velocity statistics) in three-dimensional inhomogeneous turbulence. We here consider only the basic case of a single particle in one-dimensional turbulence.

$$p(w, z, t) \propto p_a(w, z) .$$

It follows that $p_a(w, z)$ should satisfy (3), i.e.,

$$-\frac{\partial}{\partial z}(wp_a) - \frac{\partial}{\partial w}(ap_a) + \frac{1}{2}\frac{\partial^2}{\partial w^2}(b^2 p_a) = 0 . \qquad (4)$$

This is the well-mixed constraint, which restricts the selection of $a(w, z)$ and $b(w, z)$. Evidently the w.m.c. prohibits the spurious growth of order from disorder, and thus (speaking informally) is an entropy-evolution constraint.

Now, $b(w, z)$ can be obtained from the Kolmogorov inertial subrange theory as (Monin and Yaglom, 1975)

$$b(w, z) = \sqrt{C_0 \epsilon} \qquad (5)$$

or (in principle equivalently; Thomson, 1987) by

$$b(w, z) = \sqrt{\frac{2M_2}{\tau}} ; \qquad (6)$$

C_0 is a (supposedly) universal constant, here taken to be 2.0; ϵ is the rate of dissipation of the turbulent kinetic energy; M_2 $(= \sigma_w^2)$ is the variance of the vertical velocity; and τ is the Lagrangian decorrelation time scale.

The difference between the exact model and the approximate model lies in the specification of $a(w, z)$.

2.2. The exact model

If the Eulerian pdf for the vertical velocity $p_a(w, z)$ is known, $a(w, z)$ can be derived from (4) in principle as (Thomson, 1987)

$$a(w, z) = \frac{\left[\frac{\partial}{\partial w}\left(\frac{1}{2} b^2 p_a\right) + \phi\right]}{p_a} , \qquad (7)$$

where ϕ is the solution of

$$\frac{\partial \phi}{\partial w} = -\frac{\partial p_a}{\partial z} \qquad (8)$$

satisfying $\phi \to 0$ as $|w| \to \infty$. However, only for particular forms for $p_a(w, z)$ can one solve analytically for ϕ.

2.3. The moments approximation model

To avoid needing explicitly the Eulerian pdf, Kaplan and Dinar (1992, 1993) approximate $a(w, z)$ as:

$$a(w,z) = C_0(z) + C_1(z)w + C_2(z)w^2 + \\ + C_3(z)w^3 + \cdots + C_k(z)w^k + \cdots . \quad (9)$$

Substituting this expansion into the governing equation for the characteristic function of $p_a(w, z)$

$$\Theta(\theta, z) = \int_{-\infty}^{\infty} p_a(w, z)e^{iw\theta}\, \mathrm{d}w ,$$

and making use of Equation (4), we have

$$-i\frac{\partial^2\Theta}{\partial z\,\partial\theta} - i\theta\left[C_0\Theta - iC_1\frac{\partial\Theta}{\partial\theta} - C_2\frac{\partial^2\Theta}{\partial\theta^2} + \cdots \right. \\ \left. + (-1)^k i^k C_k \frac{\partial^k\Theta}{\partial\theta^k} + \cdots\right] + \frac{b^2}{2}\theta^2\Theta = 0 \quad (10)$$

(note that no summation is implied by the recurring index k).

Equation (10) indicates that satisfaction of the w.m.c. is guaranteed provided infinitely many terms in the expansion (9) are retained. However, the moments approximation method is useful only to the extent that one may truncate Equation (9) at a small number of terms: so we need to determine whether the w.m.c. remains satisfied (approximately) upon such truncation.

By repeated differentiation of (10) with respect to θ, one can obtain (on setting $\theta = 0$) a set of simultaneous equations for the coefficients C_i in terms of the moments M_i. Provided that the number of terms retained in (9) is finite, a closed solution for these coefficients in terms of a finite number of specified moments is available. For example, if we retain 5 terms (C_0, C_1, C_2, C_3 and C_4) in (9), we must differentiate (10) five times, and obtain:

$$\begin{aligned}
C_0M_0 + C_1M_1 + C_2M_2 + C_3M_3 + C_4M_4 &= \frac{\mathrm{d}M_2}{\mathrm{d}z} ,\\
C_0M_1 + C_1M_2 + C_2M_3 + C_3M_4 + C_4M_5 &= \frac{1}{2}\frac{\mathrm{d}M_3}{\mathrm{d}z} - \frac{b^2}{2}M_0 ,\\
C_0M_2 + C_1M_3 + C_2M_4 + C_3M_5 + C_4M_6 &= \frac{1}{3}\frac{\mathrm{d}M_4}{\mathrm{d}z} - b^2M_1 , \qquad (11)\\
C_0M_3 + C_1M_4 + C_2M_5 + C_3M_6 + C_4M_7 &= \frac{1}{4}\frac{\mathrm{d}M_5}{\mathrm{d}z} - \frac{3}{2}b^2M_2 ,\\
C_0M_4 + C_1M_5 + C_2M_6 + C_3M_7 + C_4M_8 &= \frac{1}{5}\frac{\mathrm{d}M_6}{\mathrm{d}z} - 2b^2M_3 ,
\end{aligned}$$

where M_k is the k-th order moment of the turbulent velocity. In general if the expansion (9) for $a(w)$ retains terms up to order w^K, then the set of simultaneous equations for the coefficients C_k ($k \leqslant K$) will involve moments as high as M_{2K}. For the case of $K = 1$, we need to assume that $\mathrm{d}M_3/\mathrm{d}z = 0$.

Our specification of the C's is slightly different from that used by Kaplan and Dinar, who made the approximation (from dimensional considerations) that $C_1 = -b^2/2M_2$. Therefore the comparisons between "exact" and "approximate" models shown in the following section do not necessarily represent comparisons to the original Kaplan–Dinar model, but rather to a modified version of it.

3. Comparison of the Exact and Approximate Models

In this section we look at several ideal turbulence systems wherein the velocity pdf (hence all moments) are known. Our object is to examine any deterioration of the moments approximation model (relative to the exact model) due to truncation (neglect of high order moments).

3.1. Gaussian Turbulence

A Gaussian velocity pdf is a satisfactory approximation in many flows (Batchelor, 1953), a familiar example being the atmospheric surface layer under neutral stratification. For Gaussian turbulence, the probability density function is

$$p_a(w, z) = \frac{1}{\sqrt{2\pi} M_2^{1/2}} \exp\left(-\frac{w^2}{2M_2}\right), \tag{12}$$

and the moments are[2]

$$M_{2n+1} = 0\,,$$
$$M_{2n} = (2n-1)!!M_2^n\,.$$

Using (12), one readily obtains the exact model (Thomson, 1987)

$$a(w, z) = -\frac{b^2}{2M_2} w + \frac{1}{2}\left(\frac{w^2}{M_2} + 1\right)\frac{\mathrm{d}M_2}{\mathrm{d}z}, \tag{14}$$

and, by using (13), exactly the same expression arises following the approximate approach,

$$C_0 = \frac{1}{2}\frac{\mathrm{d}M_2}{\mathrm{d}z}, \qquad C_1 = -\frac{b^2}{2M_2},$$
$$C_2 = \frac{1}{2M_2}\frac{\mathrm{d}M_2}{\mathrm{d}z}, \qquad C_3 = 0, \qquad C_4 = 0\,. \tag{15}$$

The above derivation shows that for Gaussian turbulence, these two methods are consistent with each other, which is not surprising since the pdf is fully defined by the first two moments.

[2] $(2n-1)!! = (2n-1)(2n-3)\ldots 5.3.1.$

3.2. Homogeneous non-Gaussian turbulence

We now examine the flow having pdf[3]

$$p_a(w) = \frac{1}{M_2^{1/2}} \exp\left[\!\left[-\left[\lambda_0 + \lambda_1 \left(\frac{w}{M_2^{1/2}}\right) + \lambda_2 \left(\frac{w}{M_2^{1/2}}\right)^2 + \right.\right.\right.$$
$$\left.\left.\left. + \lambda_3 \left(\frac{w}{M_2^{1/2}}\right)^3 + \lambda_4 \left(\frac{w}{M_2^{1/2}}\right)^4 \right]\right]\!\right], \qquad (16)$$

where the λ's are related to skewness ($S = M_3/M_2^{3/2}$) and kurtosis ($K = M_4/M_2^2$). We shall use $S = 0.65$ and $K = 3.0$ (values typical of the convective boundary layer). These constraints, plus normalization, and the specification of zero mean velocity, imply

$$\begin{aligned} &\lambda_0 = 0.9881, \quad \lambda_1 = 0.5941, \quad \lambda_2 = 0.3281, \\ &\lambda_3 = -0.2594, \quad \lambda_4 = 0.0708\,. \end{aligned} \qquad (17)$$

From Equations (7), (8), (16) and (17) it follows that the exact model is:

$$a(w) = -\frac{b^2}{2M_2^{1/2}} \left[\lambda_1 + 2\lambda_2 \left(\frac{w}{M_2^{1/2}}\right) + 3\lambda_3 \left(\frac{w}{M_2^{1/2}}\right)^2 + 4\lambda_4 \left(\frac{w}{M_2^{1/2}}\right)^3 \right], \qquad (18)$$

i.e., the approximate model (9) is actually exact provided that the C_i are given by[4]

$$\begin{cases} C_i = -\dfrac{b^2}{2} \dfrac{(i+1)\lambda_{i+1}}{M_2^{(i+1)/2}}, & (i = 0, 1, 2, 3) \\ C_i = 0 & (i \geqslant 4). \end{cases} \qquad (19)$$

Consider now the hypothetical case of a worker not privileged to know the pdf (16), who is given only a certain number of velocity moments, and who wishes to use that restricted information in the approximation (9), i.e., the information (19) is not available to this person.

Let us for convenience set $\tau = 30$ [s] and $M_2 = 1$ [m^2/s^2]. The exact model (18) becomes

$$a(w) = -0.01980 - 0.02187w + 0.02594w^2 - 0.009447w^3\,. \qquad (18')$$

Our worker knows some or all of these moments:[5]

[3] Readers may recognize this pdf as being of the form of a maximum missing information pdf. However, this pdf is used here simply as a convenient example.

[4] We are indebted to Dr. N. Dinar for noting this formula.

[5] These values for $M_5 \rightarrow M_8$ follow from (16), although from the viewpoint of our worker unaware of (16), they are simply data made available.

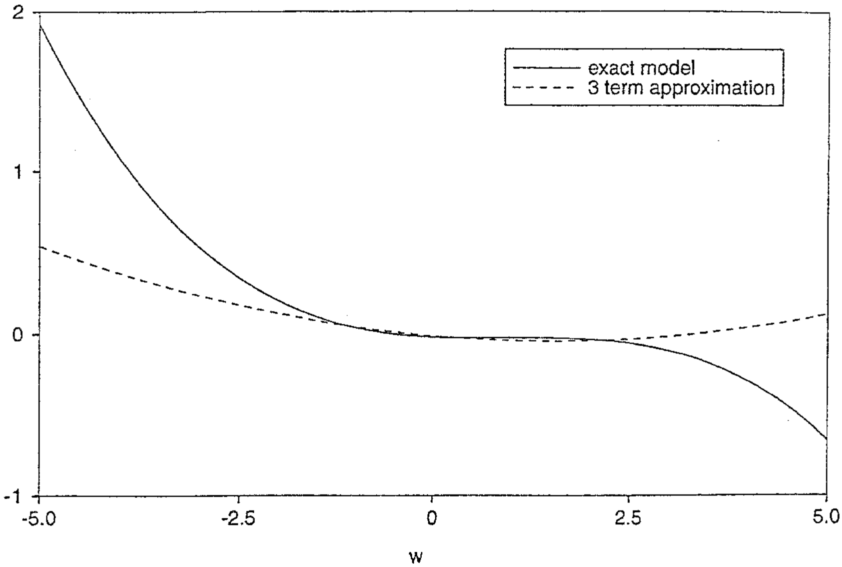

Fig. 1. Comparison of $a(w)$ in the exact model and the three-term approximation model. The flow is homogeneous and non-Gaussian.

$$\begin{aligned} &M_0 = 1, \quad M_1 = 0, \quad M_2 = 1, \quad M_3 = 0.65, \quad M_4 = 3, \\ &M_5 = 4.64, \quad M_6 = 15.03, \quad M_7 = 33.43, \quad M_8 = 100.27\,. \end{aligned} \tag{20}$$

Depending on whether $M_0 \to M_4$ or $M_0 \to M_6$ or $M_0 \to M_8$ is given, the worker will deduce (in corresponding order) that

$$a(w) = -0.01373 - 0.04226w + 0.01373w^2\,, \tag{21a}$$

$$a(w) = -0.01980 - 0.02187w + 0.02594w^2 - 0.009441w^3\,, \tag{21b}$$

$$\begin{aligned} a(w) = &-0.01980 - 0.02187w + 0.02594w^2 - \\ &- 0.009441w^3 - 9.0\ 10^{-8}w^4\,. \end{aligned} \tag{21c}$$

Small differences between coefficients in 21(b, c) and in the exact model (18′) are due to roundoff errors.

We have shown that if a worker unaware of the pdf makes use of only the moments $M_0 \to M_4$, he/she obtains a model (Equation (21a)) quite distinct from the exact model (Equation (18′)). How good or bad is the approximation? Figure 1 shows that the difference between the exact and the approximate models is quite large. The deterministic term $a(w)$ normally has the effect of returning the velocity towards its conditional mean value. The approximate model with four or more terms does have that property, but with only three terms it does not. In the latter case, $a(w)$ drives a large positive velocity even larger.

We calculated the spread of particles released at $z_s = 500\,\mathrm{m}$, into a domain

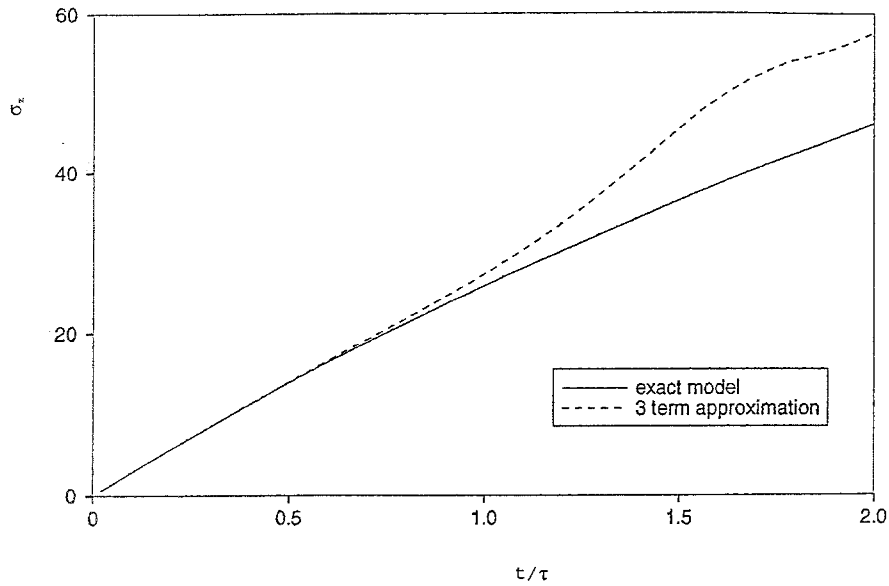

Fig. 2. The predicted standard deviation by both the exact model and the three-term approximation model in homogeneous non-Gaussian turbulence. Perfect reflection was applied at both top and bottom boundaries. 5,000 particles were released at $z_s = 500$ m with initial velocity drawn from the Eulerian velocity distribution. In calculation, $\Delta t = 0.01\tau$.

bounded by perfect reflection at $z = (0, 1000)$ m, using a time step 0.01τ. Figure 2 compares the calculated standard deviation of the particle position from the exact and the approximate model (21a) over the range of $(0, 2\tau)$. For a short flight time, the approximate model gives a satisfactory result due to memory of correct release statistics, but for $t > \tau$, it is quite wrong because the particles' flights are governed by an incorrect conditional mean acceleration $a(w)$.

Figure 3 shows that there arises a violation of the w.m.c., with regard to both position and velocity, when the moments approximation model is truncated at $K = 2$ (i.e., four moments are used, and we retain terms to order w^2 in $a(w)$). In Figure 3(a), we show that violation of the w.m.c. in position worsens as flight time t of the particles increases. For $t = \tau$, the degree of violation is not serious (due to the correct release statistics), but for later times, it becomes unacceptable. Figure 3(b), on the other hand, indicates that the pdf of the particle velocity, calculated from the moments approximation model, decays with respect to the initial pdf; in particular, at large w the probability density grows with time. This is not surprising in view of the expansion used for $a(w)$: the three-term approximation forces large w to be even larger.

Of course, the worker using approximation (21a) does not know the correct pdf (16), so would have no basis for considering the velocity pdf that results from his model (21a) as "wrong" by comparison with (16). In fact, the moments approxi-

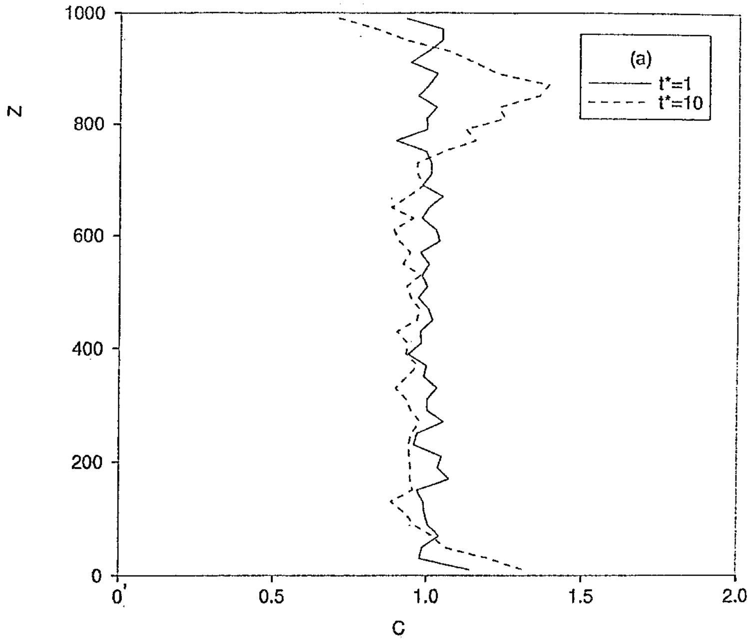

Fig. 3(a).

mation for $a(w)$, in conjunction wlth other assumptions made, may (under suitable restrictions) imply a pdf. In the present case, however (homogeneous, four specified moments, second-order polynomial), such a pdf is not implied (see Appendix). Particles in the present simulation were released with a random velocity from the "exact" pdf (16), but since the underlying moments approximation model does not imply a pdf, we should not be surprised to see that at later times, there is no pdf approaching (16).

3.3. Inhomogeneous non-Gaussian turbulence

The Eulerian probability density function for vertical velocity in the convective boundary layer (CBL) is commonly modelled (e.g., Baerentsen and Berkowicz, 1984) as bi-Gaussian,

$$p_a(w, z) = \frac{A}{\sqrt{2\pi}\sigma_A} \exp\left[-\frac{(w - w_A)^2}{2\sigma_A^2} \right] + \frac{B}{\sqrt{2\pi}\sigma_B} \exp\left[-\frac{(w + w_B)^2}{2\sigma_B^2} \right], \tag{22}$$

where $A(B)$ is the fractional area occupied by thermals (downdrafts), $w_A(w_B)$ the mean velocity within the thermals (downdrafts) and $\sigma_A(\sigma_B)$ the standard deviation of the fluctuating vertical velocity in thermals (downdrafts). As in Du *et al.* (1994), we choose to relate the parameters of (22) to the unconditional moments by

$$A = 0.4, \quad B = 0.6$$

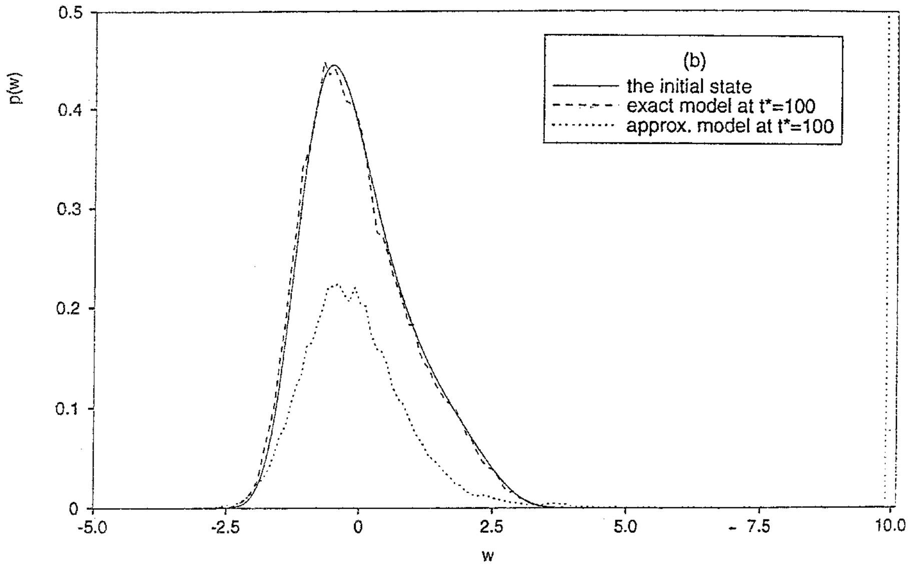

Fig. 3. (a) The evolution of the concentration distribution from an initially well-mixed profile ($C = 1$) predicted by the three term approximate model. (b) The probability density distribution of vertical velocity at $t^* = t/\tau = 100$, calculated from both the exact model and three-term approximation model. The solid line is the probability density function at $t = 0$. In the calculation, 50,000 particles were released with the "well-mixed" initial condition. In calculating the concentration distribution, perfect reflection was employed at both boundaries. In calculating the evolution of the pdf, no reflection scheme was used.

$$\begin{aligned} w_A &= M_3^{1/3}, \quad w_B = \tfrac{2}{3}M_3^{1/3}, \\ \sigma_A &= (M_2 - 0.281M_3^{2/3})^{1/2}, \quad \sigma_B = (M_2 - 0.927M_3^{2/3})^{1/2}. \end{aligned} \tag{23}$$

We assume $S = 0.65$ and $K = 3.0$, typical of values observed in the CBL. In deriving approximate models, we need higher velocity moments. From (22), (23) we get

$$\begin{aligned} &M_5 = 4.627M_2^{5/2}, \quad M_6 = 15.662M_2^3, \quad M_7 = 35.992M_2^{7/2}, \\ &M_8 = 116.438M_2^4. \end{aligned} \tag{24}$$

From (7), (8), (22) we obtain the exact model equations

$$\mathrm{d}w = \frac{-(M_2/\tau)Q + \phi}{p_a(w)}\,\mathrm{d}t + \sqrt{\frac{2M_2}{\tau}}\,\mathrm{d}\xi\,, \tag{25}$$

where

$$\phi = -\frac{A}{2}\frac{\partial w_A}{\partial z}\,\mathrm{erf}\left(\frac{w - w_A}{\sqrt{2}\sigma_A}\right) +$$

$$+\left[\sigma_A \frac{\partial \sigma_A}{\partial z} + \frac{w(w - w_A)}{\sigma_A}\frac{\partial \sigma_A}{\partial z} + w\frac{\partial w_A}{\partial z}\right]p_A +$$

$$+\frac{B}{2}\frac{\partial w_B}{\partial z}\operatorname{erf}\left(\frac{w + w_B}{\sqrt{2}\sigma_B}\right) +$$

$$+\left[\sigma_B \frac{\partial \sigma_B}{\partial z} + \frac{w(w + w_B)}{\sigma_B}\frac{\partial \sigma_B}{\partial z} - w\frac{\partial w_B}{\partial z}\right]p_B , \quad 26)$$

$$Q = \frac{(w - w_A)Ap_A}{\sigma_A^2} + \frac{(w + w_B)Bp_B}{\sigma_B^2}, \quad (27)$$

$$p_A = \frac{1}{\sqrt{2\pi}\sigma_A}\exp\left[-\frac{(w - w_A)^2}{2\sigma_A^2}\right], \quad (28)$$

$$p_B = \frac{1}{\sqrt{2\pi}\sigma_B}\exp\left[-\frac{(w + w_B)^2}{2\sigma_B^2}\right]. \quad (29)$$

Again, the approximate model equation depends on how many terms in the expansion (9) are used. If three terms are used,

$$\begin{aligned} C_0 &= -0.206\frac{b^2}{M_2^{1/2}} + 0.567\frac{\mathrm{d}M_2}{\mathrm{d}z}, \\ C_1 &= \frac{-0.634b^2 + 0.206(\mathrm{d}M_2/\mathrm{d}z)M_2^{1/2}}{M_2}, \\ C_2 &= \frac{(0.206b^2/M_2^{1/2}) + 0.433(\mathrm{d}M_2/\mathrm{d}z)}{M_2}. \end{aligned} \quad (30)$$

Using four terms,

$$\begin{aligned} C_0 &= -\frac{0.279b^2}{M_2^{1/2}} + 0.550\frac{\mathrm{d}M_2}{\mathrm{d}z}, \\ C_1 &= \frac{-0.385b^2 + 0.265(\mathrm{d}M_2/\mathrm{d}z)M_2^{1/2}}{M_2}, \\ C_2 &= \frac{(0.353b^2/M_2^{1/2}) + 0.468(\mathrm{d}M_2/\mathrm{d}z)}{M_2}, \\ C_3 &= \frac{-0.115b^2 - 0.027(\mathrm{d}M_2/\mathrm{d}z)M_2^{1/2}}{M_2^2}, \end{aligned} \quad (31)$$

while with five terms,

$$C_0 = \frac{-0.293b^2}{M_2^{1/2}} + 0.579\frac{\mathrm{d}M_2}{\mathrm{d}z},$$

$$C_1 = \frac{-0.418b^2 + 0.330(\mathrm{d}M_2/\mathrm{d}z)M_2^{1/2}}{M_2},$$
$$C_2 = \frac{(0.381b^2/M_2^{1/2}) + 0.412(\mathrm{d}M_2/\mathrm{d}z)}{M_2}, \tag{32}$$
$$C_3 = \frac{-0.097b^2 - 0.062(\mathrm{d}M_2/\mathrm{d}z)M_2^{1/2}}{M_2^2},$$
$$C_4 = \frac{(-0.008b^2/M_2^{1/2}) + 0.016(\mathrm{d}M_2/\mathrm{d}z)}{M_2^2}.$$

We computed the dispersion of tracer particles in a flow in which the profile of variance was specified as

$$M_2(z) = w_s^2\left[0.01 + \left(\frac{z}{Z_i}\right)^{2/3}\left(1 - \frac{z}{Z_i}\right)^{2/3}\right], \tag{33}$$

where w_s is the scale of vertical velocity, taken to be 1 m/s. This profile (33) is in qualitative agreement with experimental data in the CBL (Sawford and Guest, 1987; Stull, 1988). The Lagrangian decorrelation time scale was set to

$$\tau(z) = \frac{2.5M_2Z_i}{w_s^3}. \tag{34}$$

Using (34) is equivalent to taking

$$b = \left(\frac{w_s^3}{1.25Z_i}\right)^{1/2}. \tag{35}$$

Simulations were performed for point ($z_s = 500$ m) and well-mixed releases, with a timestep 0.01τ. The height of the boundary layer Z_i was 1000 m.

Figure 4 shows that the approximate models satisfactorily predict the standard deviation of the dispersing particle position, but not the mean height. The five-term approximation is not, however, superior to the four-term one.

Figure 5 shows the mean density distribution (C) at $t = 2\tau_{\max}$ (where $\tau_{\max}$ is the Lagrangian time scale at the mid-point of the computational domain) of particles released from a well-mixed initial state ($C = 1$). The four-term approximation satisfies the w.m.c. (within statistical error), but the three- and five-term approximations do not (note the accumulation of particles at the middle of the domain and the deficit near the boundaries). This suggests that using more terms does not necessarily improve the approximate model. At first glance, this seems strange. However, common sense suggests that the expansion for $a(w, z)$ terminating at the term $C_K w^K$ requires that K be odd and that $C_K < 0$; otherwise $a(w, z)$ can drive the magnitude of a large velocity even larger. For example, if $K = 4$, then a positive (negative) C_4 will force a positive (negative) velocity of large

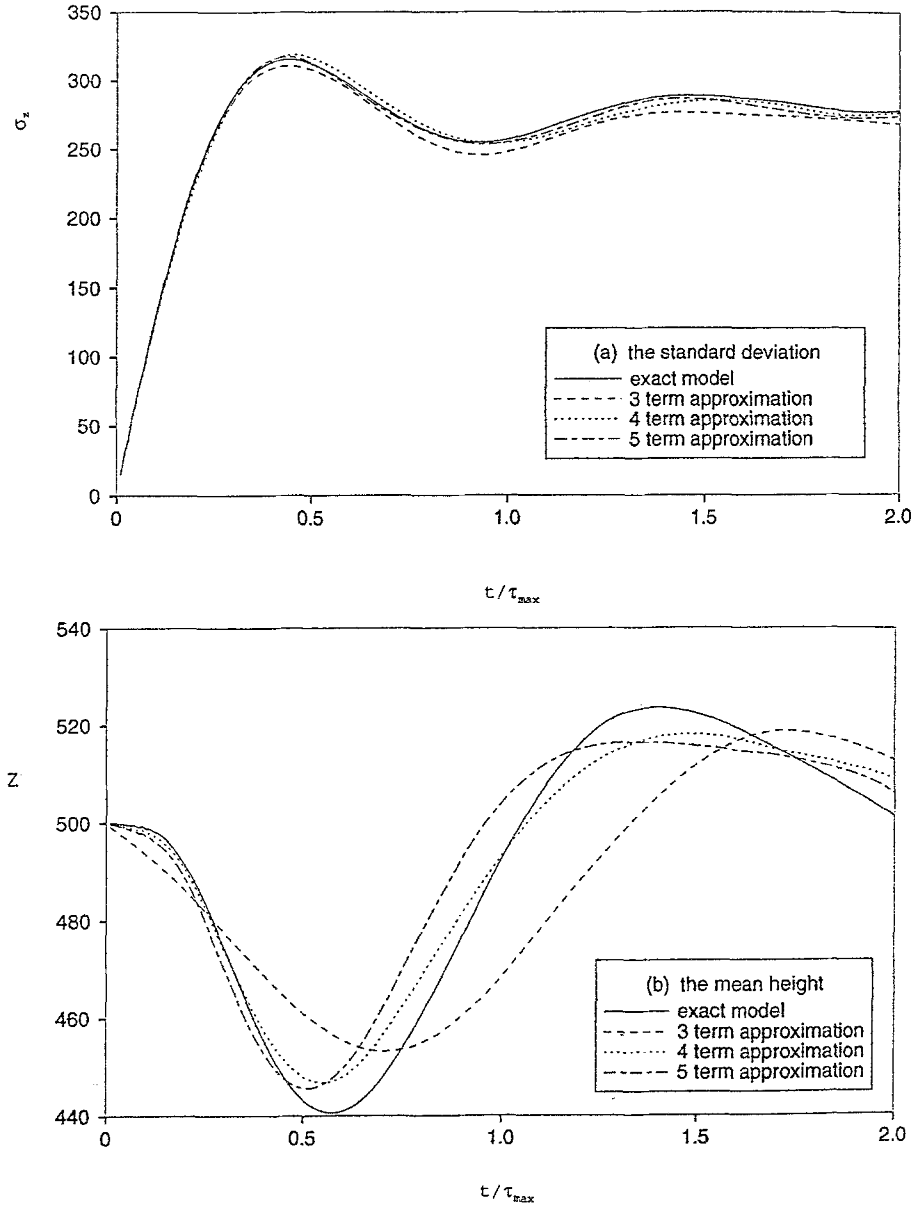

Fig. 4. (a) Comparison of the calculated standard deviation by the exact model and the approximate models in inhomogeneous non-Gaussian turbulence. The source height was $z_s = 500\,\mathrm{m}$. τ_{max} is the maximum Lagrangian time scale in the computational domain. (b) Comparison of the calculated mean height of the dispersing particles by the exact model and approximate LS models.

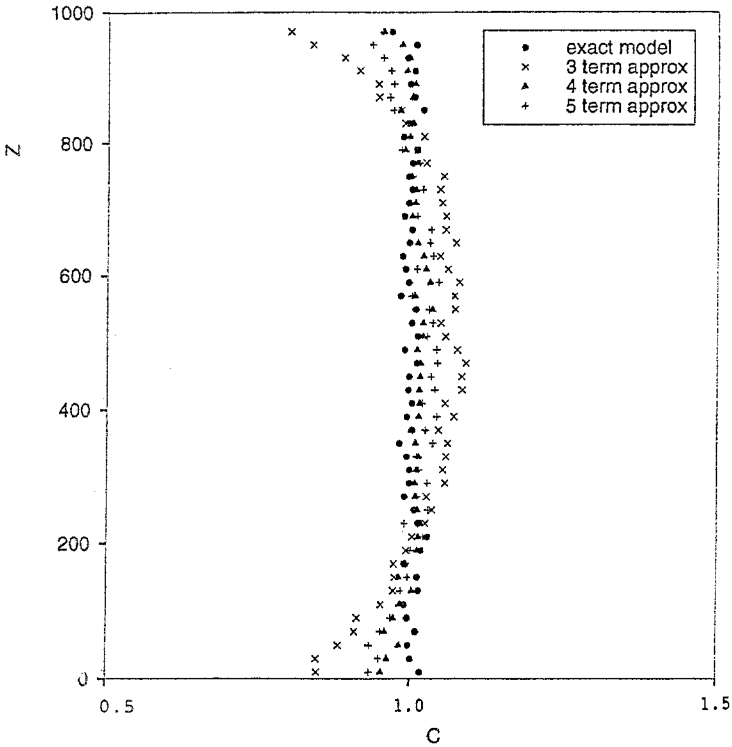

Fig. 5. The evolution of a well-mixed initial concentration profile in inhomogeneous non-Gaussian turbulence. The profiles are at $t = 2\tau_{\max}$. In calculation, 50,000 particles were released.

magnitude even farther away from its equilibrium value, $w = 0$. In the homogeneous case we studied in the last subsection, this problem was not serious because the coefficient C_4 was extremely small. In strongly inhomogeneous turbulence, C_4 may be numerically large due to the velocity variance gradient term, so that truncating at the $C_4 w^4$ term could be problematical.

The above analysis suggests that when using the moments approximation, one should truncate the expansion for $a(w)$ (in powers w^k) at an odd power ($k \leqslant K$, K odd).

4. Forming an Optimal Lagrangian Model from Partial Information on Eulerian Velocity Statistics

Rather than assuming a fully-known pdf (whose specification was not, however, available for the purpose of exploiting the Kaplan–Dinar method), we shall now examine the situation where an LS model is to be built strictly from partial information – so that one cannot, even in principle, appeal to an "exact" model as a criterion. Specifically, we shall assume that only the N lowest-order moments are known, and compare the following two models:

(i) the modified Kaplan–Dinar moments approximation model;
(ii) the well-mixed model that corresponds to the "maximum missing information" pdf (not the true pdf, which is unknown) implied by the given moments.

Model (i) is by now familiar: all information given about the Eulerian velocity is used to determine the coefficient C's of a truncated expansion for $a(w, z)$. Model (ii) begs explanation.

When one must form a pdf on the basis of partial information about a random variable, the scientifically objective choice is the pdf which is "maximally noncommittal with regard to missing information" (Jaynes, 1957). This objectivity is achieved by choosing the pdf which maximizes the functional

$$H(p) = -\int_{-\infty}^{\infty} p(w) \ln[p(w)] \, \mathrm{d}w$$

under the given constraints (this inference principle is well-known in statistics, and has already been applied in the context of LS models by Du *et al.*, 1994). Having formed this "mmi" (maximum missing information) pdf, one may then (in principle, though not necessarily easily) derive the corresponding well-mixed LS model.

4.1. Optimal trajectory model from $N = 2$ given moments

Suppose we are given the mean and variance of the Eulerian velocity. We are not entitled to assume that the Eulerian pdf is Gaussian.

The mmi pdf in this case (not the actual) pdf, which remains unknown) is Gaussian (Du *et al.*, 1994). Therefore the LS model obtained from the mmi principle and the w.m.c. is simply the model (14) given earlier (Section 3.1).

If we employ the moments approximation in this case, we are limited to the expansion:

$$a(w, z) = C_0 + C_1 w \,, \tag{36}$$

and we obtain

$$C_0 = \frac{\mathrm{d}M_2}{\mathrm{d}z}, \qquad C_1 = -\frac{b^2}{2M_2} \,. \tag{37}$$

Clearly this model is quite different from (14) or (15). We suspect that this is not a well-mixed model in the inhomogeneous case. We have been unable to prove this point. But in random flight experiments (using the inhomogeneous turbulence profiles of Section 3), the initial well-mixed distribution was retained much more closely by the mmi model (14) than by the moments approximation model (36),

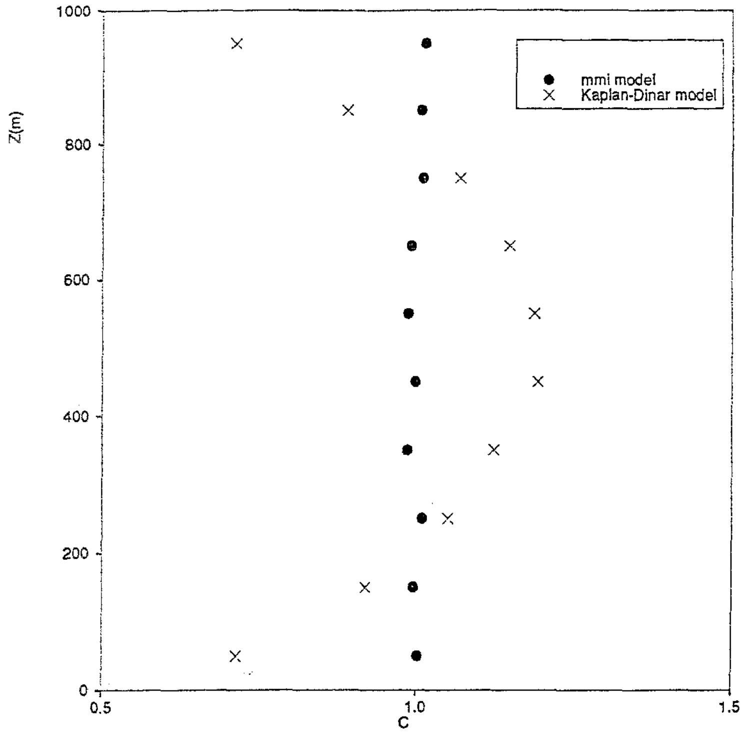

Fig. 6. The evolution of a well-mixed initial concentration profile ($C = 1$) in inhomogeneous turbulence when only two velocity moments are specified. The profiles are at $t = 5\tau_{max}$. In calculation, 50,000 particles were released.

(37), as shown in Figure 6. This must be qualified by stating that: (a), we did not know the correct initial velocity statistics for the moments approximation model; and (b), implementing perfect reflection at the boundaries implied an unavoidable (though arguably minor) violation of the w.m.c. (see Wilson and Flesch, 1993) by both models.

In this case, our exploitation of the mmi principle to build an LS model from partial information has yielded a more-rigorous model than does the moments approximation (36).

4.2. Optimal trajectory model from $N = 4$ given moments

In this case, given the four lowest-order moment constraints, the mmi pdf is (Du *et al.*, 1994)

$$p(w, z) = \exp\left(-\sum_{k=0}^{4} \lambda_k(z) w^k \right),$$

where the $\lambda_k(z)$s are determined by the four known moments and the normalization condition. Following Thomson (1987), the corresponding well-mixed LS model is

$$a(w, z) = -\frac{M_2}{\tau} \sum_{k=1}^{4} k\lambda_k(z) w^{k-1} + \\ + \left[\sum_{k=0}^{4} \frac{d\lambda_k(z)}{dz} \int_{-\infty}^{w} w'^{k+1} p(w', z)\, dw' \right] \Big/ p(w, z) . \tag{38}$$

We refer to this as the mmi model.

The two methods under consideration use exactly the same information about the Eulerian velocity distribution, but proceed on different routes to obtain the LS model equation. Which is better? To answer this, we simulated dispersion from a continuous point source at height $Z_s = 0.24Z_i$ in the CBL (of depth Z_i), adopting the velocity statistics $M_2(z)$, $M_3(z)$ and $\tau(z)$ that were previously used for the same purpose by Luhar and Britter (1989), plus a supplementary (and justified; see Du *et al.*, 1994) assumption that $M_4 = 3.0M_2^2$.

Figure 7 compares predictions of the two models for the contours of cross-wind integrated concentration (CWIC), and may be compared with the corresponding contours of the convection tank experiment of Willis and Deardorff (1978; their Figure 4). The mmi model seems superior to the modified Kaplan-Dinar model. In Figure 8 we compare predictions of the alongwind profile of ground-level CWIC. Again, the mmi model gives the better prediction. In particular, at (what should be) suitably large downwind distances ($X \sim 4$), the CWIC predicted by the modified Kaplan–Dinar model is not well mixed.

5. Conclusion

From a practical viewpoint, the concept of an "exact" Eulerian velocity pdf is absurd (as any experimentalist would confirm), and the Kaplan–Dinar aspiration to build a Lagrangian stochastic model from realistic, partial knowledge of the turbulence (a few low-order velocity moments) is appropriate.

However, what is involved here is a statistical inference problem, and the Kaplan–Dinar approach may not be the best one. We have shown that a danger of the Kaplan–Dinar approach is that one may obtain a random flight algorithm that fails the well-mixed condition (does not keep an initially well-mixed tracer well-mixed). On the basis of our findings, we suggest that a better alternative to the Kaplan–Dinar approximation is to construct from the known velocity statistics the maximum missing information probability density function: then by the usual procedure (Thomson, 1987) derive the corresponding well-mixed trajectory model.

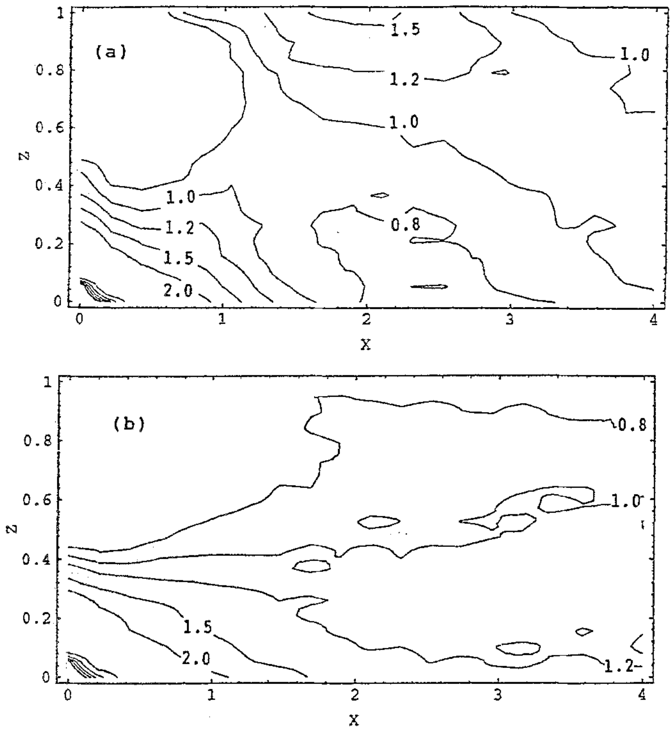

Fig. 7. Comparison of the CWIC contours in the X–Z plane predicted by (a) the mmi model and (b) the modified Kaplan–Dinar model in the CBL. X is dimensionless downwind distance defined as $X = xw_s/UZ_i$, and $Z = Z_s/Z_i$.

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Appendix. Eulerian velocity pdf implied by the moments approximation

Thomson (1987) has shown that the Eulerian velocity pdf $p_a(w, z)$ must be a solution of the Fokker–Planck equation that corresponds to (any) suitable model for the evolution of particle velocity (the well-mixed condition referred to earlier). We note that if expansion (9) for the model coefficient $a(w, z)$ is substituted into the FP equation, one may obtain an Eulerian pdf that is derived consistently from the principal assumptions made (Markovian evolution; model must be well-mixed;

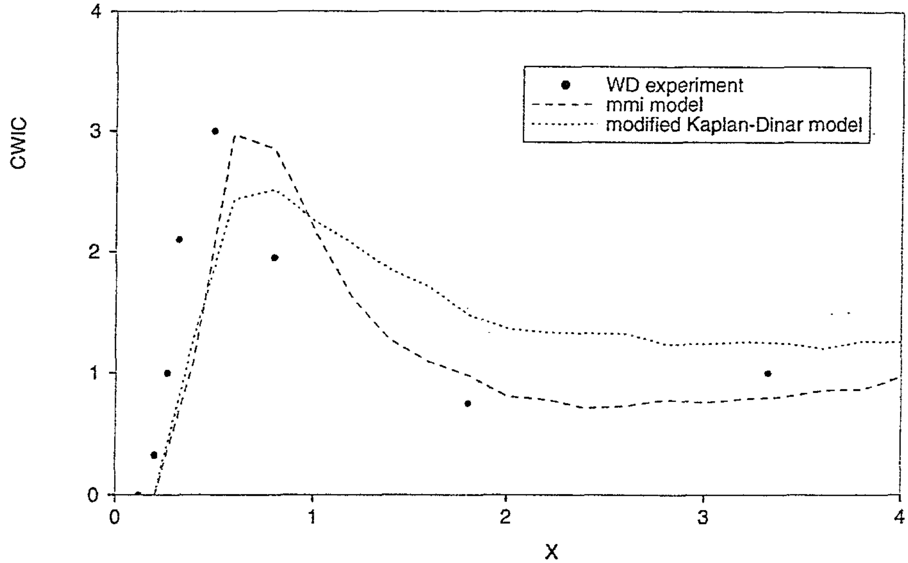

Fig. 8. Comparison of calculated ground-level CWIC from both the mmi model and the modified Kaplan–Dinar model with Willis and Deardorff's water tank experiment. The well-mixed value (which should occur at large X) is CWIC = 1.

coefficient b independent of w; power series expansion for $a(w, z)$). In the case of homogeneous turbulence, the solution to the FP equation is:

$$p_a(w) = \exp\left[\frac{2}{b^2}\left(C_* + C_0 w + \frac{C_1}{2} w^2 + \cdots \frac{C_K}{K+1} w^{K+1}\right)\right]. \tag{A1}$$

If K is even, this solution (Equation (A1)) is unbounded, and so not a pdf.

On the other hand, if K is odd, the solution (Equation (A1)) is of the form of an mmi (maximum missing information) pdf (for a detailed description of the mmi pdf, the reader is referred to Du *et al.*, 1994). However, determining the coefficients $C_0, C_1 \ldots C_K$ of the modified Kaplan–Dinar expansion (and of the above pdf) requires knowledge of $2K$ velocity moments,[6] whereas the pdf (A1) is exactly the mmi pdf corresponding to a smaller number (K) of given velocity moments. C_* can be determined by the normalization condition or any one of the given moments.

It is seen, then, that the modified KD model, in effect, may imply a pdf. Presumably the principle of consistency of approximation requires that the part-

[6] The original Kaplan–Dinar approach requires $(2K - 1)$ moments plus an assumption (concerning C_1) in the one-dimensional case.

icles of a modified *KD* simulation be released with a random velocity from that pdf.

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