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PROBABILITY DENSITY FUNCTIONS FOR VELOCITY IN THE CONVECTIVE BOUNDARY LAYER, AND IMPLIED TRAJECTORY MODELS

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Abstract—When a probability density function (pdf) is to be formed on the basis of incomplete information, the "maximum missing information" (mmi) pdf (Jaynes, *Phys. Rev.* **106,** 620–630, 1957) is theoretically preferable. We compare the performance of Lagrangian stochastic (LS) models of vertical dispersion in the convective boundary layer, satisfying Thomson's (*J. Fluid Mech.* **180,** 529–556, 1987) well-mixed condition, that derive from the often-used bi-Gaussian pdf (eg. Weil, *J. atmos. Sci.* **47,** 501–515, 1990) and from the mmi pdf. The bi-Gaussian based LS model, which we tailor to reproduce velocity moments to fourth order, is less complex than the corresponding mmi based model, and gives similar (good) predictions, which are arguably slightly superior (as regards agreement with convection tank data) to those stemming from the original bi-Gaussian based model (Luhar and Britter, *Atmospheric Environment* **23,** 1911–1924, 1989), wherein knowledge of the kurtosis was forsaken.

Key word index: Probability density function (pdf), maximum missing information (mmi) pdf, bi-Gaussian pdf, Lagrangian stochastic model.

1. INTRODUCTION

When taking advantage of Thomson's (1987) well-mixed condition (w.m.c.) in designing Lagrangian stochastic (LS) models of trajectories in turbulent flow, we must specify the Eulerian probability density function (pdf) of the fluctuating velocity. Except in idealized flows, that pdf is not exactly known, so it is usual practise to assume a pdf, guided by experimental evidence. Flesch and Wilson (1992) showed that adding increasingly numerous moment constraints, to shape an *ad hoc* pdf so as to describe highly non-Gaussian turbulence, can result in deteriorating agreement between simulation and measurement. It is clear then that criteria are needed in formulating the pdf, and we here investigate using the "maximum missing information" (mmi) pdf.

Though our point is general, we will discuss the choice of a pdf in the context of modelling vertical dispersion in the convective boundary layer (CBL). Up to now, the most widely used pdf for the CBL has been the bi-Gaussian (a linear combination of two Gaussian functions), proposed by Baerentsen and Berkowicz (1984), supported by atmospheric observations (Quintarelli, 1990), and used to build a well-mixed LS model by Luhar and Britter (1989) and Weil (1990). Our considerations lead to an LS model that performs slightly better than its predecessors.

2. CRITERIA IN CONSTRUCTING A PDF

Assume we require to choose a pdf $p(x)$ for a variable x, which is random on the range $(-\infty, \infty)$. According to information theory (Jaynes, 1957), $p(x)$ should:

a. reflect all the information we actually have; and
b. maximize

$$H(p) = -\int_{-\infty}^{\infty} p(x)\ln p(x)\,\mathrm{d}x. \qquad (1)$$

$H(p)$ quantifies "missing information" (Baierlein, 1971; Guiasu, 1977), i.e provides a numerical measure of the amount of additional information that is needed to determine the pdf correctly and uniquely. It may be surprising that the "amount of missing information", on first sight a qualitative concept, can be given a unique quantitative measure. We will attempt no formal justification, but perhaps the following words might help. We reduce our uncertainty about the pdf with the help of information given us (e.g. moment constraints). However, uncertainty remains, because an infinite number of pdfs are consistent with the given (finite number of) constraints. The principle of scientific objectivity dictates that we be maximally *uncommitted* about what we do not know concerning the pdf, and the requirement that $p(x)$ maximizes $H(p)$ enforces that principle: by satisfying (*b*) in our choice of $p(x)$, we are "maximally non-committal with respect to missing information" (Jaynes, 1957).

Now, we seek a pdf $p(x)$ that maximizes $H(p)$, subject to the constraints:

$$\int_{-\infty}^{\infty} x^j p(x)\,\mathrm{d}x = \mu_j \quad (j=1,2,\ldots,N) \tag{2}$$

and the normalization condition $\int_{-\infty}^{\infty} p(x)\,\mathrm{d}x = 1$. We set $\mu_1 = 0$, without loss of generality. Introducing appropriate Lagrange multipliers $\{\lambda_k\}_{k=0}^{N}$ (Swokowski, 1979), one seeks maximization of the functional $H^* = H^*(p)$ defined from

$$H^*(p) = -\int_{-\infty}^{\infty} p(x)\ln p(x)\,\mathrm{d}x + (\lambda_0 - 1)\times\left(1-\int_{-\infty}^{\infty} p(x)\,\mathrm{d}x\right) + \sum_{k=1}^{N}\lambda_k\left(\mu_k - \int_{-\infty}^{\infty} x^k p(x)\,\mathrm{d}x\right).$$

Functional variation with respect to the unknown pdf, $p(x)$

$$\frac{\delta H^*(p)}{\delta p(x)} = 0 \tag{3}$$

yields the following mmi pdf:

$$p(x) = \exp\left(-\sum_{k=0}^{N}\lambda_k x^k\right). \tag{4}$$

Where the $N+1$ unknown Lagrange multipliers are determined from the normalization condition and the given moments by the implicit relationships

$$\exp(\lambda_0) = \int_{-\infty}^{\infty}\exp\left(-\sum_{k=0}^{N}\lambda_k x^k\right)\mathrm{d}x \equiv Z \tag{5}$$

and

$$\mu_j = \frac{1}{Z}\int_{-\infty}^{\infty} x^j \exp\left(-\sum_{k=1}^{N}\lambda_k x^k\right)\mathrm{d}x \qquad j=1,2,\ldots,N. \tag{6}$$

If $N>2$, an analytical solution is impossible, because the numerator of equation (6) involves an integral which cannot in general be expressed in terms of elementary functions. We infer that:

(I) If we seek the mmi pdf for a random variable x defined on $(-\infty, \infty)$, subject to constraints (i.e. available information) of the usual form (namely, a set of moment constraints), our search can succeed only if we have an *even* number of moment constraints.

(II) From equation (4), to ensure the pdf reproduces the known moments and vanishes for very large $|x|$, we must require $\lambda_N > 0$, where N (necessarily even, from (I)) is the highest order imposed moment constraint.

3. PDFS FOR VERTICAL VELOCITY (w) IN THE CBL

We assume available the information that:

$$\langle w\rangle = 0$$
$$\langle w^3\rangle = S\langle w^2\rangle^{3/2}$$
$$\langle w^4\rangle = 3.0\,\langle w^2\rangle^2$$

where S is the skewness. A value of about 3 for the kurtosis is supported by data from the Boulder Atmospheric Observatory (see Fig. 1), and by aircraft observations (Hanna, 1982).

3.1. *The mmi pdf*

The mmi pdf, which is in principle to be preferred, is:

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

At each of 10 heights within the CBL, we determined numerically the set of values $(\lambda_0, \lambda_1, \ldots, \lambda_4)$ consistent with the four velocity–moment constraints, and the normalization condition.

3.2. *Bi-Gaussian pdf*

Baerentsen and Berkowicz (1984; hereafter BB) proposed to use in the CBL the pdf

$$p(w,z) = \frac{A}{\sqrt{2\pi}\,\sigma_A}\exp\left[-\frac{(w-w_A)^2}{2\sigma_A^2}\right] + \frac{B}{\sqrt{2\pi}\,\sigma_B}\exp\left[-\frac{(w+w_B)^2}{2\sigma_B^2}\right] \tag{7}$$

where A and B are the fractional areas occupied by thermals and the compensating downdrafts, and $w_A(w_B)$ and $\sigma_A(\sigma_B)$ are the mean and the standard deviation of the fluctuating vertical velocity within thermals (downdrafts). Making no use of information

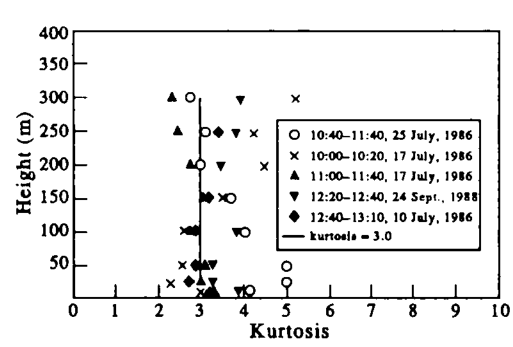

Fig. 1. Kurtosis of the vertical velocity during unstable stratification at the Boulder Atmospheric Observatory tower. The solid line is $K=3.0$, the kurtosis for Gaussian turbulence.

on the kurtosis, but assuming

$$\sigma_A = w_A, \quad \sigma_B = w_B \tag{8}$$

BB obtained the parameters:

$$\begin{aligned} \sigma_B = w_B &= [(\langle w^3\rangle^2 + 8\langle w^2\rangle^3)^{1/2} - \langle w^3\rangle]/4\langle w^2\rangle \\ \sigma_A = w_A &= \langle w^2\rangle / 2w_B \\ A = w_B/(w_A + w_B), &\quad B = w_A/(w_A + w_B). \end{aligned} \tag{9}$$

Luhar and Britter (1989) used equations (9) in their LS model. Weil (1990), assuming (rather than equation (8)) that $\sigma_A/w_A = \sigma_B/w_B = R$ (where R is an arbitrary constant taken as 1.5), used similar expressions. Note that in view of the discussion of Section 2, it is not possible to construct the mmi pdf corresponding to the bi-Gaussian equations (9).

One is quite at liberty to specify the parameters of the bi-Gaussian otherwise than equation (9). We are interested to see whether the bi-Gaussian can approximate the mmi pdf, *that corresponds to the given information*. The mmi pdf, as stated, made use of the known kurtosis: so that information, if the comparison is to be fair, must be brought to bear in fitting the bi-Gaussian.

Invoking knowledge of the kurtosis, we require to solve

$$\begin{aligned} &A + B = 1 \\ &Aw_A - Bw_B = 0 \\ &A(\sigma_A^2 + w_A^2) + B(\sigma_B^2 + w_B^2) = \langle w^2\rangle \\ &A(3w_A\,\sigma_A^2 + w_A^3) - B(3w_B\,\sigma_B^2 + w_B^3) = \langle w^3\rangle \\ &A(3\sigma_A^4 + 6w_A^2\,\sigma_A^2 + w_A^4) + B(3\sigma_B^4 + 6w_B^2\,\sigma_B^2 + w_B^4) = \langle w^4\rangle. \end{aligned} \tag{10}$$

Now assumption (8) is not supported by experimental data (Lenschow and Stephens, 1982), so we close the set of equations (10) by instead assuming

$$A = 0.4. \tag{11}$$

This is supported by many experiments (Hunt *et al.*, 1988; Fritsch and Businger, 1973; among others), but is not valid as stratification tends towards the neutral condition. Under this assumption, and provided $S \leqslant 1.12$ (which is usually the case; LeMone, 1990), the solution is

$$\begin{aligned} &A = 0.4, \quad B = 0.6 \\ &w_A = \langle w^3\rangle^{1/3}, \quad w_B = (2/3)\,\langle w^3\rangle^{1/3} \\ &\sigma_A = (\langle w^2\rangle - 0.280\,\langle w^3\rangle^{2/3})^{1/2} \\ &\sigma_B = (\langle w^2\rangle - 0.927\,\langle w^3\rangle^{2/3})^{1/2}. \end{aligned} \tag{12}$$

Figure 2 compares the mmi pdf with the two bi-Gaussian pdfs, for $S = 0.2$, 0.65 and 1.0. Not surprisingly, our alternate bi-Gaussian pdf generally approximates the mmi pdf better than does the BB bi-Gaussian pdf (pay particular attention to the pdf near the mode, whose value greatly affects the mean concentration field; Hunt *et al.*, 1988).

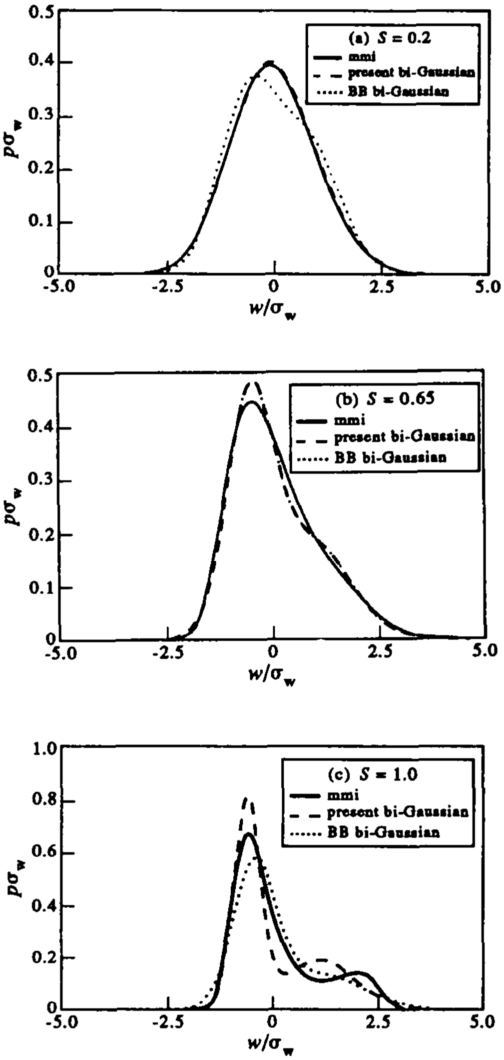

Fig. 2. Comparison of the "correct" pdf which maximizes the missing information with both the present and Baerentsen and Berkowitz bi-Gaussian pdfs for (a) $S = 0.2$; (b) $S = 0.65$, and (c) $S = 1.0$.

4. LS MODELS FOR THE CBL, FROM BI-GAUSSIAN AND MMI PDFS

The well-mixed LS model corresponding to the Baerentsen and Berkowicz bi-Gaussian pdf was derived by Luhar and Britter (1989), to whom the reader may refer. A similar derivation, based on our (alternatively fitted) bi-Gaussian, yields a similar model:

$$\mathrm{d}w = \left[-\frac{\langle w^2\rangle}{\tau} Q + \phi \right] \frac{\mathrm{d}t}{p(w, z)} + \left(\frac{2\langle w^2\rangle \mathrm{d}t}{\tau} \right)^{1/2} \mathrm{d}\mu \tag{13}$$

(terms have the same meaning as in LB). Q and ϕ are given by:

$$Q = \frac{(w - w_A)\,Ap_A}{\sigma_A^2} + \frac{(w + w_B)\,Bp_B}{\sigma_B^2} \tag{14}$$

$$\begin{aligned}\phi = &-\frac{A}{2}\frac{\partial w_A}{\partial z}\operatorname{erf}\left(\frac{w-w_A}{\sqrt{2}\sigma_A}\right)\\ &+\left[\sigma_A\frac{\partial \sigma_A}{\partial z}+\frac{w(w-w_A)}{\sigma_A}\frac{\partial \sigma_A}{\partial z}+w\frac{\partial w_A}{\partial z}\right]P_A \\ &+\frac{B}{2}\frac{\partial w_B}{\partial z}\operatorname{erf}\left(\frac{w+w_B}{\sqrt{2}\sigma_B}\right)\\ &+\left[\sigma_B\frac{\partial \sigma_B}{\partial z}+\frac{w(w+w_B)}{\sigma_B}\frac{\partial \sigma_B}{\partial z}-w\frac{\partial w_B}{\partial z}\right]P_B .\end{aligned} \quad (15)$$

In the case of the mmi pdf, we obtain the model equation

$$\mathrm{d}w = a(w,z)\,\mathrm{d}t + \left(\frac{2\langle w^2\rangle}{\tau}\mathrm{d}t\right)^{1/2}\mathrm{d}\mu \quad (16)$$

where

$$a(w,z) = -\frac{\langle w^2\rangle}{\tau}\sum_{k=1}^{4} k\,\lambda_k(z)\,w^{k-1} + \left[\sum_{k=0}^{4}\frac{d\lambda_k(z)}{\mathrm{d}z}\int_{-\infty}^{w} w^{k+1}\,p(w,z)\,\mathrm{d}w\right]\Big/ p(w,z). \quad (17)$$

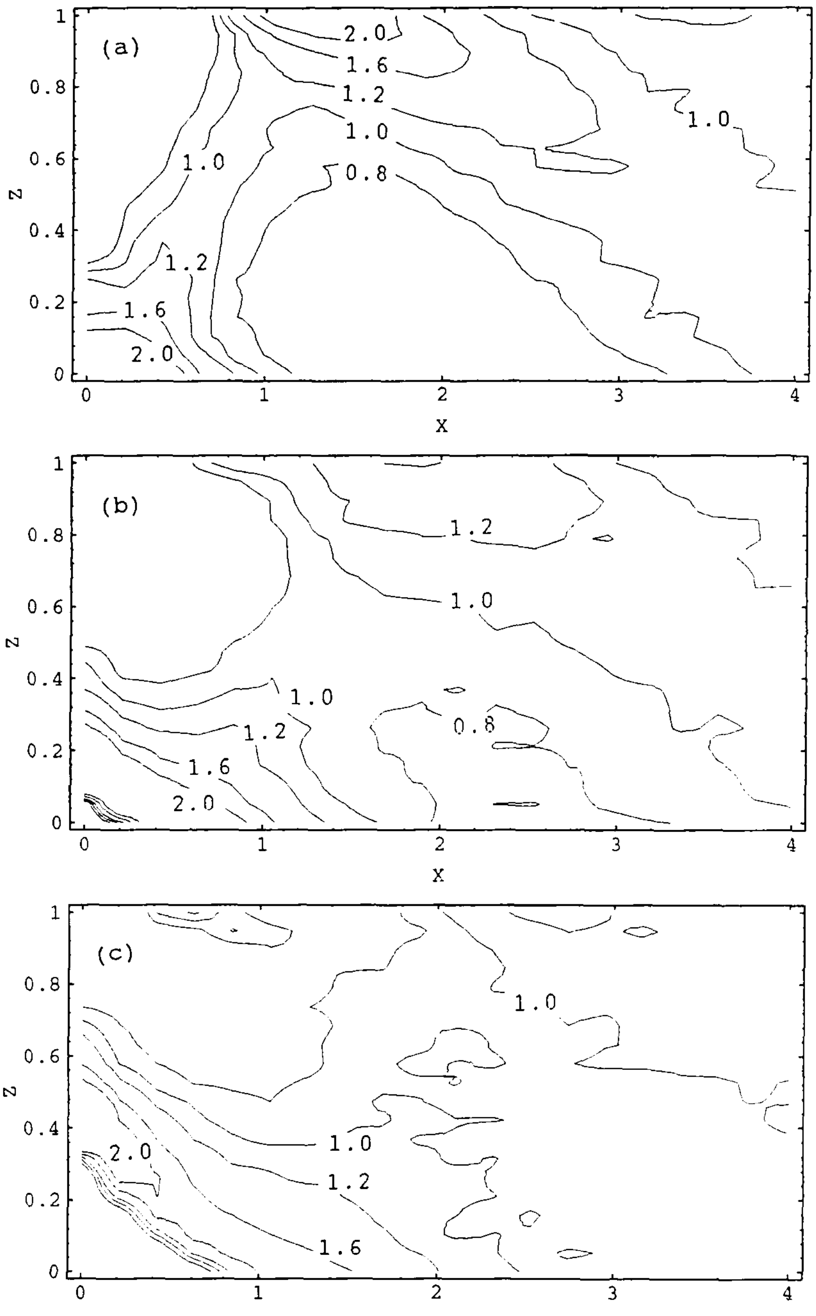

Fig. 3. Prediction of LS model corresponding to the mmi pdf for the CWIC distribution in the CBL for three release heights: (a) $Z_s/Z_i = 0.067$; (b) $Z_s/Z_i = 0.24$; and (c) $Z_s/Z_i = 0.49$.

We adopted exactly the same turbulence statistics for the CBL as did LB, and we carried out LS trajectory simulations, using both the bi-Gaussian-based models and the mmi model, for tracer particles released at source heights $Z_s = 0.067$, 0.24 or 0.49; Z_i (where Z_i is the CBL depth). Perfect reflection was imposed at the top and bottom boundaries, and the time step was taken to be 0.01 τ. The model based on the mmi pdf consumed at least an order of magnitude more computer time than the bi-Gaussian model.

The mmi-based model and our bi-Gaussian based model produce fields of crosswind integrated concentration (CWIC) that are almost identical, but different from the prediction that stems from the BB bi-Gaussian (Figs 3 and 4). A feature we for the moment focus on, familiar from the convection tank

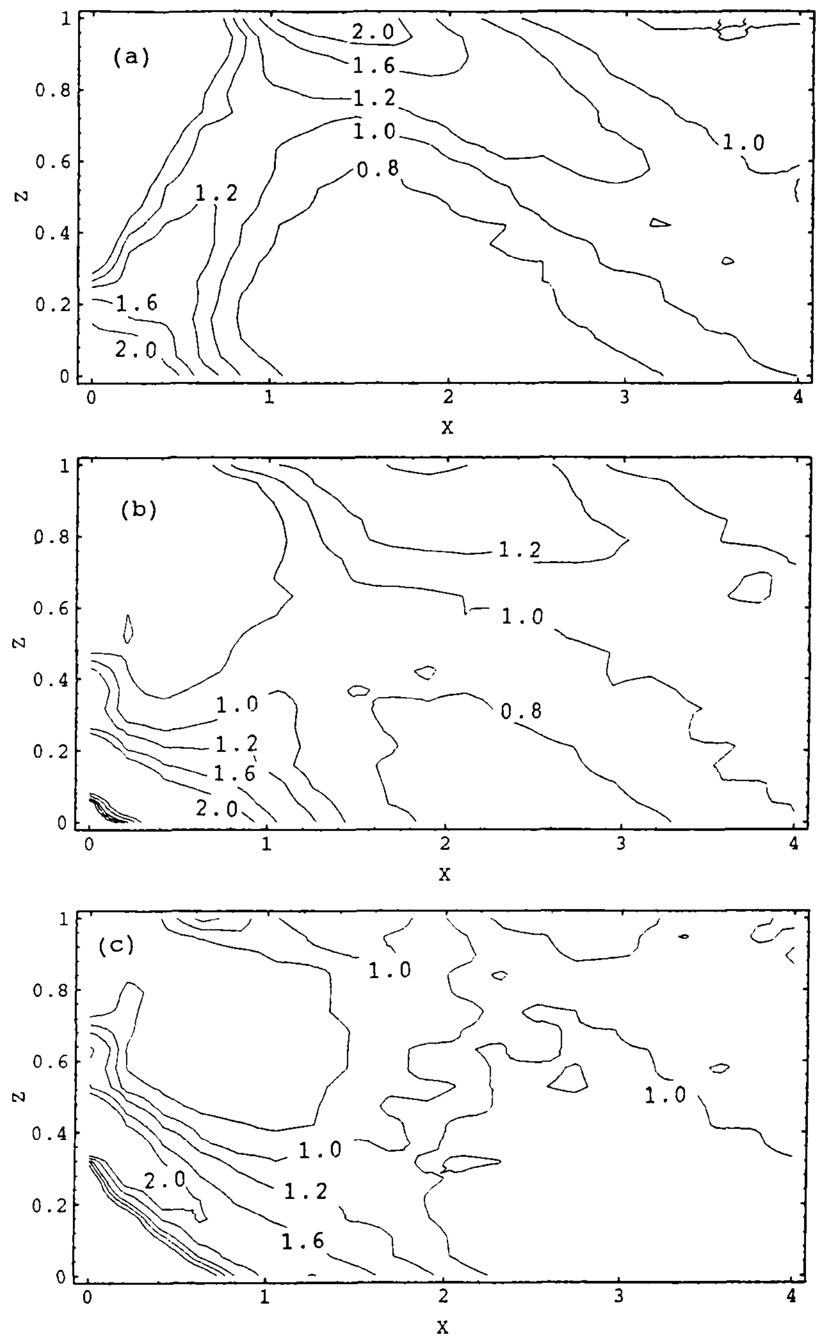

Fig. 4. Prediction of LS model corresponding to the present bi-Gaussian pdf for the CWIC distribution in the CBL for three release heights: (a) $Z_s/Z_i = 0.067$; (b) $Z_s/Z_i = 0.24$; and (c) $Z_s/Z_i = 0.49$.

Table 1. Location X_{max} of maximum surface concentration according to LS models, and; WD water-tank experiment; Lamb LES/LS simulation; CONDORS field experiment

			Model			
Z_s	Convection tank WD	Field CONDORS	LES/LS LAMB*	LS LB	LS MMI†	LS present bi-Gaussian
0.24	0.4		0.6	0.78	0.6 ± 0.2	0.68
0.32		0.8–0.9		1.03	0.8 ± 0.2	0.89
0.49	0.8		1.2	1.54	1.4 ± 0.2	1.33

* Slightly different release heights were used in Lamb's works: 0.26 corresponding to 0.24 of the WD and 0.50 to 0.49 of the WD.

† For the mmi LS model, the X_{max} is obtained from the calculated CWIC distribution rather than from equation (18). However, we infer that the mmi LS model and the LS model derived from the present bi-Gaussian pdf yield the same X_{max} because the mode of velocity in these two pdfs are nearly same.

experiments of Willis and Deardorff (1978, 1981; hereafter WD), is that the locus of the maximum concentration descends until it reaches the ground, causing the maximum ground-level concentration to occur much closer to the source than it would in un-skewed turbulence (of otherwise equal properties). For a given source height, the distance X_{max} to the point of maximum ground-level concentration can be estimated by (Misra, 1982; Li and Briggs, 1987)

$$X_{max} = \int_{h^*/Z_i}^{Z_s/Z_i} \frac{dz/Z_i}{w_B/w_*} \qquad (18)$$

where X_{max} is non-dimensional on the translational velocity U and the convective time scale Z_i/w_*. Table 1 gives X_{max}, according to the present LS models; the WD water-tank experiments; a simulation by Lamb (1978, 1982) of particle trajectories in the turbulent field generated by Deardorff's (1974) large-eddy simulation; and the CONDORS field experiment (Briggs, 1989). We conclude that —in regard to X_{max}— the mmi model (and its more economical relative, our alternatively fitted bi-Gaussian) is superior to the model based on the BB bi-Gaussian. A weakness of the latter pdf is that it implies

$$\frac{\partial w_B}{\partial \langle w^3 \rangle} = -\frac{(\langle w^3 \rangle^2 + 8\langle w^2 \rangle^3)^{1/2} - \langle w^3 \rangle}{4\langle w^2 \rangle (\langle w^3 \rangle^2 + 8\langle w^2 \rangle^3)^{1/2}} < 0$$

for $\langle w^2 \rangle \neq 0$. The magnitude of the mean velocity in the downdrafts decreases with increasing $\langle w^3 \rangle$, and so takes its maximum value at $\langle w^3 \rangle = 0$. The BB bi-Gaussian model makes x_{max} *increase* with increasing skewness, contradicting the water-tank simulations. In our alternately fitted bi-Gaussian, the mean velocity in the thermals and downdrafts is determined by the third order moment only, or by skewness, $\langle w^3 \rangle / \langle w^2 \rangle^{3/2}$, for given velocity variance.

Returning to Fig. 4, overall, the LS models simulate the CWIC distribution in the lower CBL quite well (compare our results with fig. 7 of WD, 1976; fig. 4 of WD, 1978; and fig. 4 of WD, 1981). We note, however, an overprediction of the mean concentration in the upper CBL, particularly near the top boundary (the LB simulation shows the same discrepancy). We satisfied ourselves that this feature of the simulations is not due to the small (< 10%) increase in CBL depth over the period of each tank experiment, nor to detrainment of tracer out of the mixed layer (to address the latter possibility we used partial, rather than perfect, reflection at the top boundary). Possibly the velocity statistics we (and others) have adopted poorly represent the actual flow in and near the interfacial layer. That the maximum CWIC line does not impinge on the CBL top (as shown by the WD physical experiments, Lamb's (1982) numerical experiments and the CONDORS field experiments) suggests a mechanism for repelling tracer. However, on applying the LS model to the case $Z_s/Z_i = 0.75$, we get a high CWIC tongue which reaches the CBL top and is reflected back.

5. CONCLUSION

Although it is not possible to be conclusive on the basis of comparison with experimental evidence, we suggest on the basis of the foregoing that Lagrangian stochastic models of CBL dispersion should be based on the maximum missing information pdf for vertical velocity, the latter based on the first four Eulerian velocity moments (assumed given). A bi-Gaussian based model is practically as good, when fitted as we have shown here (to reproduce kurtosis). These details improve the prediction of the location of maximum ground-level concentration.

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