



An efficient Lagrangian stochastic model of vertical dispersion in the convective boundary layer

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Abstract

We consider the one-dimensional case of vertical dispersion in the convective boundary layer (CBL) assuming that the turbulence field is stationary and horizontally homogeneous. The dispersion process is simulated by following Lagrangian trajectories of many independent tracer particles in the turbulent flow field, leading to a prediction of the mean concentration. The particle acceleration is determined using a stochastic differential equation, assuming that the joint evolution of the particle velocity and position is a Markov process. The equation consists of a deterministic term and a random term. While the formulation is standard, attention has been focused in recent years on various ways of calculating the deterministic term using the well-mixed condition incorporating the Fokker–Planck equation. Here we propose a simple parameterisation for the deterministic acceleration term by approximating it as a quadratic function of velocity. Such a function is shown to represent well the acceleration under moderate velocity skewness conditions observed in the CBL. The coefficients in the quadratic form are determined in terms of given turbulence statistics by directly integrating the Fokker–Planck equation. An advantage of this approach is that, unlike in existing Lagrangian stochastic models for the CBL, the use of the turbulence statistics up to the fourth order can be made without assuming any predefined form for the probability distribution function (PDF) of the velocity. The main strength of the model, however, lies in its simplicity and computational efficiency. The dispersion results obtained from the new model are compared with existing laboratory data as well as with those obtained from a more complex Lagrangian model in which the deterministic acceleration term is based on a bi-Gaussian velocity PDF. The comparison shows that the new model performs well. © 1999 Elsevier Science Ltd. All rights reserved.

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1. Introduction

In a completely developed turbulent flow, such as the convective boundary layer (CBL), the joint evolution of

velocity and position of an individual fluid particle can be reasonably regarded as a Markovian stochastic process (Monin and Yaglom, 1975). Experimental observations indicate that the vertical turbulence in the CBL is highly inhomogeneous and skewed whereas the horizontal turbulence can be considered to be Gaussian (Willis and Deardorff, 1976, 1978, 1981).

Here we consider the one-dimensional case of vertical dispersion in the CBL assuming that the turbulent field is

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stationary and horizontally homogeneous. Under these conditions, the motion of independent fluid particles in the vertical direction (z) can be represented by the following stochastic differential equations (Thomson, 1987):

$$\begin{aligned} dw(t) &= a(w, z)dt + [C_o\varepsilon(z)]^{1/2}dW, \\ dz(t) &= w(t)dt, \end{aligned} \quad (1)$$

where w is the vertical velocity of a particle, C_o is a universal constant, $\varepsilon(z)$ is the ensemble-average rate of dissipation of turbulent kinetic energy, and dW are the increments of a Wiener process with zero mean and variance dt . The deterministic acceleration term $a(w, z)$ is a function of turbulence statistics and is derived from the following Fokker–Planck equation incorporating the well-mixed condition (Thomson, 1987):

$$\begin{aligned} w \frac{\partial P_E(w, z)}{\partial z} &= - \frac{\partial [a(w, z)P_E(w, z)]}{\partial w} \\ &+ \frac{C_o\varepsilon(z)}{2} \frac{\partial^2 P_E(w, z)}{\partial w^2}, \end{aligned} \quad (2)$$

where $P_E(w, z)$ is the (Eulerian) probability density function (PDF) of the vertical turbulent velocity (w) at a given height z .

Eq. (2) provides a relationship between the function $a(w, z)$ and the Eulerian statistical characteristics of the flow field, the latter represented by the probability distribution P_E . A natural and rigorous approach to the problem of determining $a(w, z)$, common to most Lagrangian stochastic dispersion models, consists of solving Eq. (2) by assuming an analytical expression for P_E that satisfies moment constraints and is in agreement with available data. For instance, the representation of P_E by a weighted sum of two Gaussian distributions has been used for several models (e.g., Baerentsen and Berkowicz, 1984; Luhar and Britter, 1989):

$$P_E(w, z) = A(z)P_A(w, z) + B(z)P_B(w, z), \quad (3)$$

where P_A and P_B are the velocity Gaussian PDFs around the mean positive velocity and the mean negative velocity, respectively, and the weights $A(z)$ and $B(z)$ can be associated to the probabilities of occurrence of positive and negative turbulent velocities. The PDF represented by Eq. (3) contains six unknown parameters, and the system of six equations required to determine them can be written in a closed form if the first five Eulerian moments of the velocity are known. However, this approach, although theoretically viable, presents some practical limitations, mainly because it does not provide an analytical solution (e.g. Tassone et al., 1994), but also because of the difficulties in obtaining accurate estimates of the higher order moments. Therefore, several closures have been proposed in the literature to obtain analytical solutions for the PDF parameters and to avoid the use of higher order moments (e.g. Weil, 1990; Luhar et al., 1996).

Generally, the models derived by the bi-Gaussian approximation (3) provide results that are in very good agreement with experiment, and also the physical characterization of the terms in (3) leads to well-founded closure assumptions, directly and quite simply linked to the physics of the process.

A different approach leads to the model we propose in this paper. We do not make any assumption about the form of the PDF, but only require the first four Eulerian moments of the velocity to provide information on the statistical properties of the turbulence. This is done by assuming that $a(w, z)$ is a quadratic function of the velocity, and then deriving the function coefficients using the Fokker–Planck Eq. (2). This representation has the advantage of a much better computational efficiency due to its algebraic simplicity. However, for highly skewed PDFs, this approach leads to some errors in the concentration distribution at large times, although the near-source dispersion remains correct.

The same expression for the acceleration can be obtained by expanding the acceleration as a power series in the velocity, and then truncating the series at second order. Kaplan and Dinar (1993) gave the general expression for the power series, and determine the series coefficients using the moments of the Eulerian PDF. Du et al. (1994) tested the power series expression for the acceleration truncated at orders as high as 4 in the one-dimensional case for homogeneous and inhomogeneous non-Gaussian turbulence, and discussed the effects of the approximations on the deviations from the well-mixed profile.

2. The model

We assume that the acceleration is a function of the velocity as follows:

$$a(w, z) = \alpha(z)w^2 + \beta(z)w + \gamma(z), \quad (4)$$

where the three unknown parameters $\alpha(z)$, $\beta(z)$ and $\gamma(z)$ are determined from the Fokker–Planck Eq. (2), as discussed below. The conjecture that a quadratic functional form for the acceleration could suitably represent the main mechanisms of Lagrangian turbulent dispersion relies on the consideration that such a form is the exact result for the case of Gaussian turbulence (Thomson, 1987); it is therefore natural to assume that the flexibility of this polynomial form could well adapt to conditions other than Gaussianity. Of course, we also expect that if the statistical characteristics of the flow field deviate strongly from Gaussianity, the acceleration (4) may not provide the correct description of the flow.

The system of equations that determines the parameters of the acceleration in Eq. (4) can be obtained by multiplying Eq. (2) successively by powers of w , and then integrating over the velocity. The system involves the

functions $\alpha(z)$, $\beta(z)$ and $\gamma(z)$, the Eulerian moments of w and their derivatives with respect to z :

$$\alpha(z)\overline{w^{n+1}} + \beta(z)\overline{w^n} + \gamma(z)\overline{w^{n-1}} = \frac{1}{n} \frac{\partial \overline{w^{n+1}}}{\partial z} - \frac{n-1}{2} C_o \varepsilon(z) \overline{w^{n-2}} \quad n = 1, \dots, N. \quad (5)$$

Since the turbulence is not homogeneous in the vertical direction, the Eulerian moments $\overline{w^n}$ and their corresponding derivatives depend on the position z .

Eq. (5), evaluated for $n = 1, 2$ and 3 , provides the expressions for the coefficients in Eq. (4):

$$\alpha(z) = \frac{(1/3)\partial \overline{w^4}/\partial z - \overline{w^3}/(2\overline{w^2}) [\partial \overline{w^3}/\partial z - C_o \varepsilon(z)] - \overline{w^2} \partial \overline{w^2}/\partial z}{\overline{w^4} - \overline{w^3}^2/\overline{w^2} - \overline{w^2}^2}, \quad (6a)$$

$$\beta(z) = \frac{1}{2\overline{w^2}} \left[\frac{\partial \overline{w^3}}{\partial z} - 2\overline{w^3}\alpha(z) - C_o \varepsilon(z) \right], \quad (6b)$$

$$\gamma(z) = \frac{\partial \overline{w^2}}{\partial z} - \overline{w^2}\alpha(z). \quad (6c)$$

Therefore, the acceleration is *completely* defined if the first four Eulerian moments of the velocity are known. The model allows for an independent choice for the analytical expression of the moments, eliminating the relation between kurtosis and skewness implied by sev-

eral closure assumptions for models with a bi-Gaussian PDF (e.g. Tassone et al., 1994; Luhar et al., 1996). Furthermore, Eqs. (6) show that the model reduces to the standard Gaussian form (as given in Thomson, 1987) when skewness and kurtosis tend to their Gaussian values, i.e., 0 and 3, respectively.

3. Model application

In this paper, we use the following analytical expressions for the second and third moments of the vertical

velocity in the CBL:

$$\frac{\overline{w^2}}{w_*^2} = a_1 + a_2 \left(\frac{z}{z_i} \right)^{2/3} \left(1 - \frac{z}{z_i} \right)^{4/3}, \quad (7a)$$

$$\frac{\overline{w^3}}{w_*^3} = a_3 \left(\frac{z}{z_i} \right) \left(1 - \frac{z}{z_i} \right)^2, \quad (7b)$$

where w_* is the convective velocity, z_i the mixed layer depth, and the coefficients a_1 , a_2 and a_3 are equal to 0.05, 1.7 and 1.1, respectively. These profiles are based on the experimental data shown in Fig. 1. There is a considerable scatter in the data and it is possible to choose other values for the coefficients, as discussed later.

As used by Luhar et al. (1996), we take the value of the kurtosis (K) to be equal to 3.5 [i.e., $\overline{w^4} = 3.5(\overline{w^2})^2$] and $\varepsilon = 0.4w_*^3/z_i$. The kurtosis value was based on the results from experiments using a saline water tank described by Hibberd and Sawford (1994) whereas the value of ε was based on some large eddy simulation results and field data (Luhar and Britter, 1989; Weil, 1990).

The exact value of the universal constant C_o is uncertain with various estimates obtained by different approaches ranging between 2 and 7. However, there seems to be a consensus for using a value close to 2 for models of dispersion in convective conditions (see e.g. Rotach et al., 1996 and references therein). Accordingly, we assume $C_o = 2$ in the present study.

The acceleration $a(w, z)$ given in Eq. (4) as a function of velocity, is plotted in Fig. 2 for three different heights z/z_i . Although the shape of this function is highly sensitive to the profiles of the velocity moments employed, the acceleration provided by both the present model and the Luhar–Britter (LB) model has the same qualitative behaviour for the range of velocity with highest probability, i.e. $|w/w_*| \leq 1$.

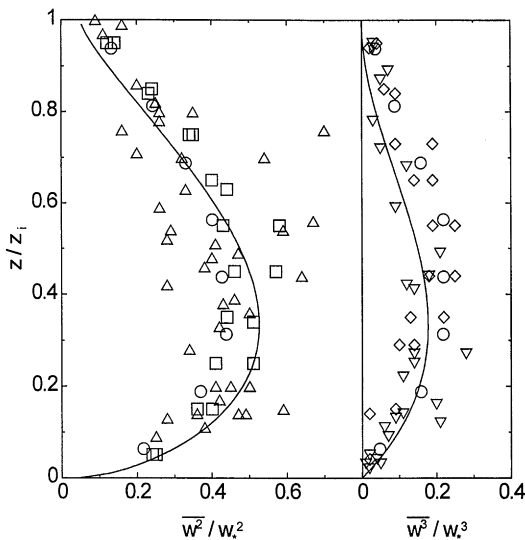


Fig. 1. Profiles of the second ($\overline{w^2}/w_*^2$) and third ($\overline{w^3}/w_*^3$) moments of the vertical velocity. Experimental data of (∇) Lenschow et al. (1980); (\circ) Luhar et al. (1996); (\diamond) Willis, from Baerentsen and Berkowicz (1984); (\square) Willis and Deardorff (1974); (\triangle) Young (1988). The solid lines are the profiles represented by Eqs. (7).

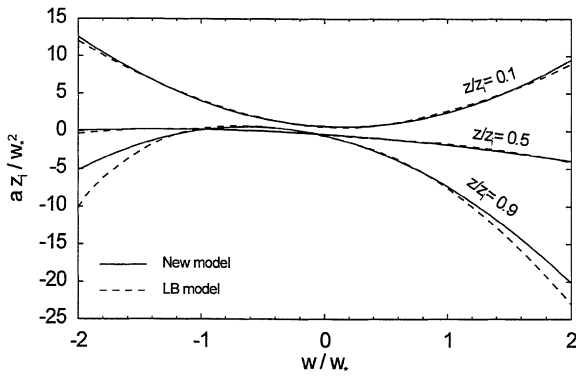


Fig. 2. Dimensionless acceleration z_i/w_*^2 as a function of velocity at 3 heights in the CBL. LB is the Luhar–Britter model.

The dispersion simulations were performed for three source heights, for which data are available from a series of experiments of Willis and Deardorff (1976, 1978, 1981). The distribution of the initial velocity of the particles was taken equal to the Eulerian velocity distribution at that height; therefore, assuming the bi-Gaussian distribution (3) to be a good approximation of the Eulerian field, the initial velocities were chosen by sampling this PDF represented by expression (3) as described in Luhar and Britter (1989). For each simulation a total of 2×10^4 particles were released and followed until a non-dimensional travel time $T = tw_*/z_i = 6$ with a time step $\Delta t = 0.01\tau(z)$, where

$$\tau(z) = \frac{2w^2}{C_o\epsilon(z)} \tag{8}$$

is the Lagrangian time scale. The particles were perfectly reflected at the boundaries; this is appropriate because of zero skewness there. The LB model with the new closure assumption described in Luhar et al. (1996) was also run for the same conditions to compare with our new model results.

3.1. Dispersion results

By applying Ito’s formula to Eq. (1), the theoretical behaviour of the mean and variance of particle heights near the source can be determined by the relations (Hunt, 1985; Thomson, 1987):

$$\overline{z(t)} = z_s + \frac{1}{2} \frac{\partial w^2}{\partial z} \Big|_{z_s} t^2 + O(t^3), \tag{9a}$$

$$\overline{(z(t) - z_s)^2} = w^2 \Big|_{z_s} t^2 + \frac{1}{2} \left(\frac{\partial w^3}{\partial z} \Big|_{z_s} - \frac{C_o\epsilon}{3} \right) t^3 + O(t^4), \tag{9b}$$

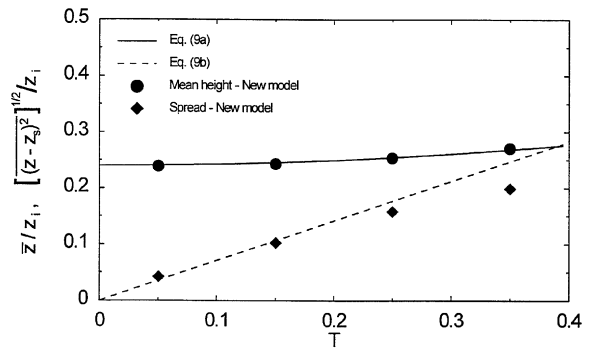


Fig. 3. Dimensionless mean particle height and spread (standard deviation) at small values of T for the source height $z_s/z_i = 0.24$. Comparison of new model with exact result given by Eqs. (9).

where z_s is the source height. These relations are independent of the approximations used to determine the acceleration term, and only assume the validity of Eqs. (1). Therefore, a first test of consistency for our model is the comparison between the results of simulations near the source with the expressions (9). Fig. 3 shows the excellent agreement at small T for both the dimensionless mean particle height \bar{z}/z_i and particle spread $[(z - z_s)^2]^{1/2}/z_i$ for the source height $z_s/z_i = 0.24$.

The non-dimensional mean particle height and spread obtained using the new model are plotted in Fig. 4a–c and Fig. 5a–c, respectively, for the source heights $z/z_i = 0.067, 0.24$ and 0.49 . Also shown are the results obtained by the LB model, along with the data from the water tank experiments of Willis and Deardorff (1976, 1978, 1981). The models show good agreement with each other and compare well with the laboratory data. However, more significant is the fact that the computational time for the present model was only a quarter that for the LB model because of the much simpler form of the acceleration term.

Fig. 6a–c presents the contour plots of the non-dimensional crosswind-integrated concentration ($\overline{C^y}$) obtained from our model for the three source heights. The contour plots obtained by Willis and Deardorff (1976, 1978, 1981) in their tank experiments are shown in Fig. 6d–f (as replotted by Hurley and Physick, 1993) and the simulations by the LB model in Fig. 6g–i. The dimensions of the cells are the same for both models, i.e. $\Delta T = 0.1, \Delta z/z_i = 0.05$. The dynamics of the dispersion is satisfactorily represented by both models including the existence of regions with counter-gradient flux (Sawford and Guest, 1987).

The ground-level concentrations shown in Fig. 7a–c indicate that the new model agrees well with the LB model but underestimates the experimentally observed peaks by 10–15% for the source heights at $0.24z_i$ and $0.49z_i$.

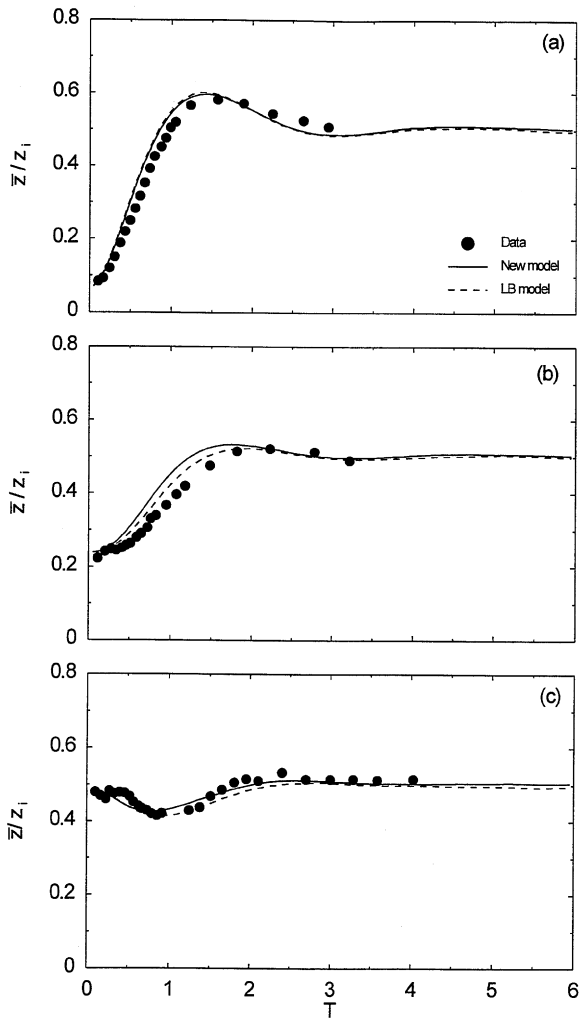


Fig. 4. Dimensionless mean particle height for source height (z_s/z_1): (a) 0.067, (b) 0.24 and (c) 0.49. New model compared with Luhar-Britter model and data of Willis and Deardorff (1976, 1978, 1981).

3.2. Limitation on skewness in the model

During tests with various fits to the experimental data in Fig. 1, it was found that the new model did not give a well-mixed concentration distribution at large times if the value of skewness was large. With increasing skewness, the near-source characteristics of the concentration field do not change, but the “well-mixed” concentration in the regions close to the boundaries is found to fall below the value in the middle of the CBL. Because the turbulence is inhomogeneous, one cannot find an exact relationship between the parameterisation of the skewness and the error affecting the asymptotic concentration profile. However, as a simple criterion for estimating the

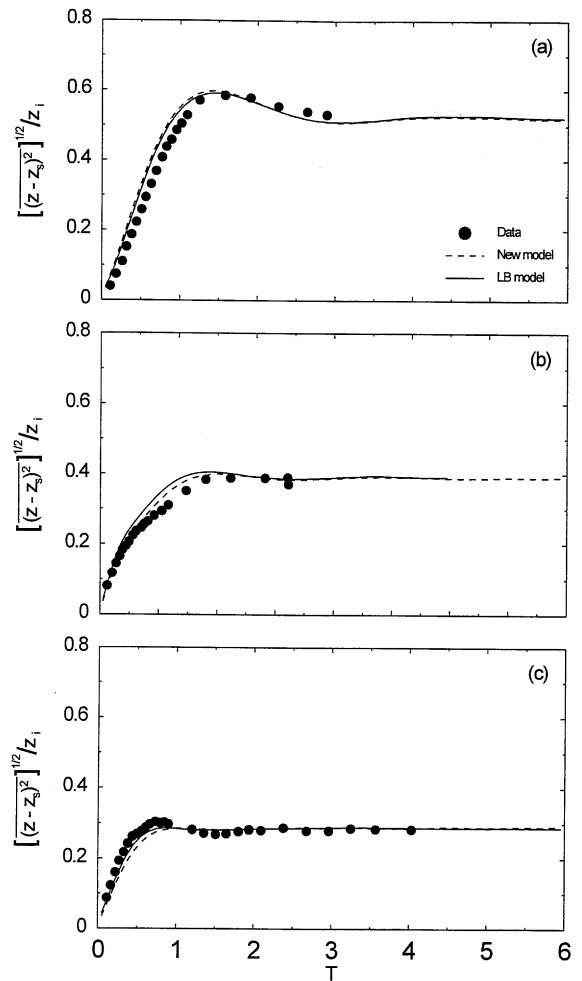


Fig. 5. Dimensionless mean particle spread for source height (z_s/z_1): (a) 0.067, (b) 0.24 and (c) 0.49. New model compared with Luhar-Britter model and data of Willis and Deardorff (1976, 1978, 1981).

accuracy of the computations we evaluated the average over the boundary layer height of the root mean squares of the error from the well-mixed concentration (C^y), at a non-dimensional time T equal to 6, as a function of the maximum skewness of the parameterised moments. The results are shown in Fig. 8. The skewness provided by the relations (7) with coefficients $a_1 = 0.05$, $a_2 = 1.7$ and $a_3 = 1.1$ defined at the start of Section 3 does not exceed a value 0.43; thus the errors in the well-mixed profile are negligible for the model results shown so far. For higher values of the skewness the concentration distribution becomes more unmixed in the regions close to the boundaries. This indicates that the polynomial form for the acceleration (4) is not suitable for such skewness values. Nevertheless, it should be noted that skewness values in the range 0.4–0.6 provide a good fit to observed data in

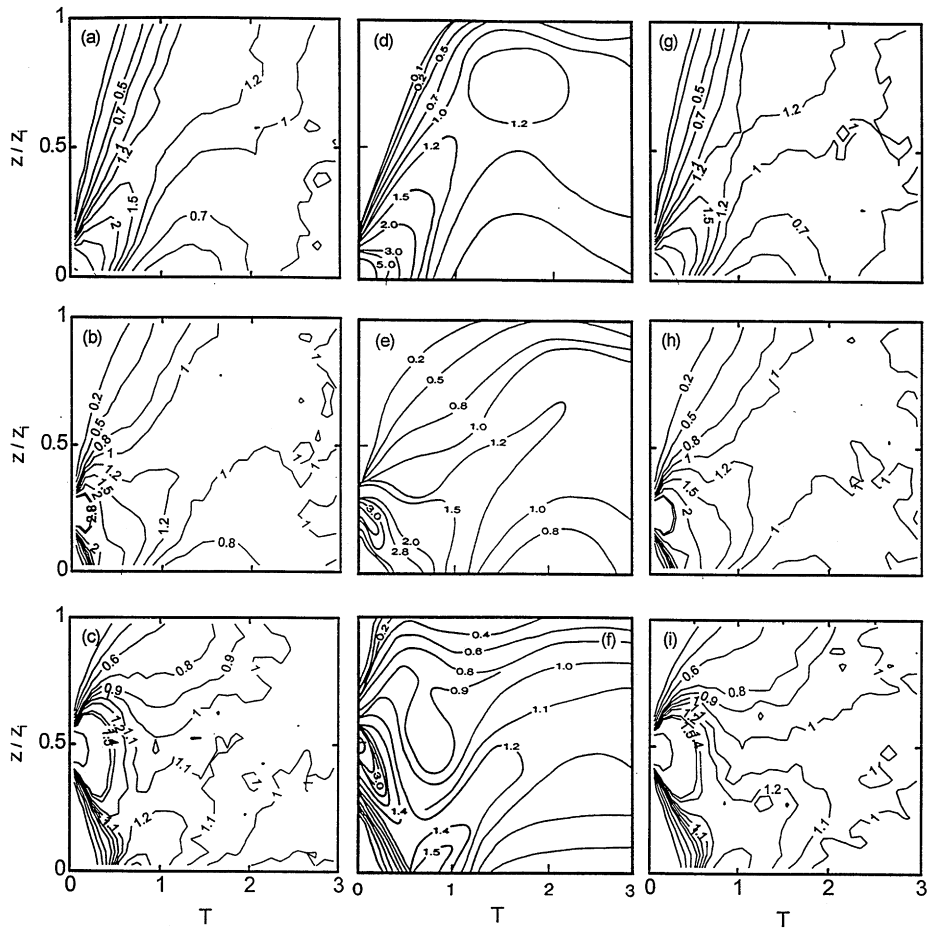


Fig. 6. Contours of the dimensionless crosswind-integrated concentration predicted by the new model (left), measured by Willis and Deardorff (1976, 1978, 1981) (center) and predicted by the Luhar-Britter model (right) for the source height (z_s/z_i) = 0.067 (top), (z_s/z_i) = 0.24 (center) and (z_s/z_i) = 0.49 (bottom).

the CBL with only minor errors in the “well mixed” region.

3.3. Comparisons of PDFs

The results in Figs. 4–7 for the average plume height, dispersion and crosswind-integrated concentration field, indicate that the particles are well mixed after $T \approx 6$. Therefore, the numerical approximation to the Eulerian PDF for the vertical velocity can be computed by sampling the particle velocity field at various heights at this time. Fig. 9a–f compare our new model PDFs obtained at six levels in the CBL with the laboratory PDFs of Luhar et al. (1996) and those obtained by the LB model. Both models underestimate the mode of the PDF, essentially because of the choice for the second moment (solid

line in Fig. 1), which is higher than the laboratory measurements across the middle region of the boundary layer. We tested the ability of the model to match the experimental PDFs with a different choice of the coefficients in Eqs. (7) for the moments: we assigned to the coefficients a_1 , a_2 and a_3 the values 0.05, 1.4 and 1.5, respectively, in order to have a closer fit to the laboratory moment data (open circles in Fig. 1). These coefficients (referred to as the second set) lead to a maximum variance ($\overline{w^2}$) of 0.44, and to a maximum skewness (S) of 0.75. Although this value of skewness produces problems in the “well mixed” concentration fields, the dot-dash line in Fig. 9a–f shows that with the second set of coefficients, the model is in better agreement with the experimental data as far as the PDF modes are concerned.

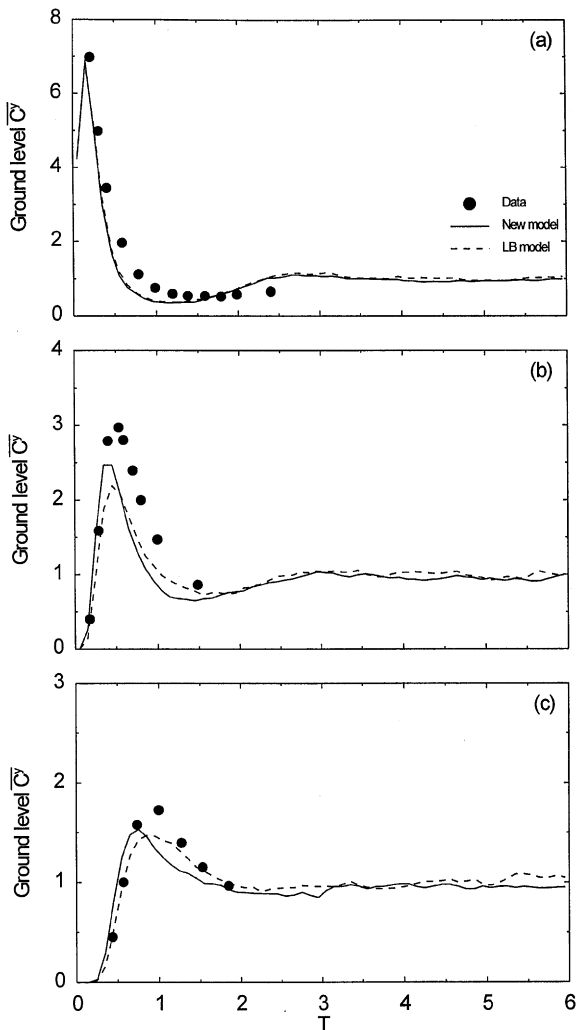


Fig. 7. Dimensionless crosswind-integrated ground level concentrations for source height (z_s/z_i): (a) 0.067, (b) 0.24 and (c) 0.49. Circles—laboratory results of Willis and Deardorff (1976, 1978, 1981).

3.4 Kolmogorov–Smirnov test

In order to evaluate the accuracy of the numerical computation of the PDF we applied the Kolmogorov–Smirnov (K–S) test (see e.g. Wilks, 1995) to the data sets. The test consists of comparing the data of two cumulative distribution functions against one another, under the null hypothesis that they were drawn from the same distribution: after calculating the K–S statistic, defined as the maximum value of the absolute difference between two cumulative distribution functions, we calculated the significance level of the statistic, under the hypothesis

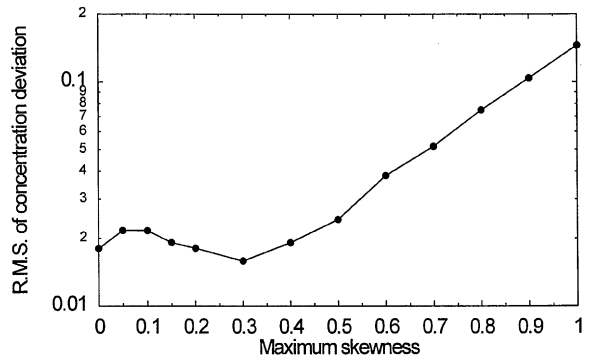


Fig. 8. Vertical average of the root mean squares of the error from the well-mixed concentration (at $T = 6$) as a function of the maximum skewness of the moment profiles.

that the compared data sets are drawn from the same distribution. A large percentage significance level means that the null hypothesis is quite likely to be true, i.e. the two compared cumulative distributions are not significantly different from each other. Fig. 10 shows the significance levels for the various pairs of data sets compared. The PDFs calculated by the new model and the LB model compare reasonably well with the experimental data. The agreement of the new model with the data is better in the central part of the boundary layer than near the boundaries. Using the second set of coefficients (with $S = 0.75$) produces worse agreement between the model PDFs and the laboratory PDFs, which is related to the problems in the concentration field caused by the higher skewness.

4. Conclusions

We have considered the one-dimensional case of vertical dispersion in the convective boundary layer assuming that the turbulence field is stationary and horizontally homogeneous, and that the evolution of the particle velocity and position is a Markov process, governed by a stochastic differential equation. We propose a simple parameterisation for the deterministic acceleration term by approximating it as a quadratic function of velocity. Such a function is shown to represent well the acceleration under moderate velocity skewness conditions observed in the CBL. The coefficients in the quadratic form are assumed to be height dependent and are determined in terms of given turbulence statistics by directly integrating the Fokker–Planck equation.

An advantage of this approach is that, unlike in existing Lagrangian stochastic models for the CBL, the use of the turbulence statistics up to the fourth order can be made without assuming any predefined form for the

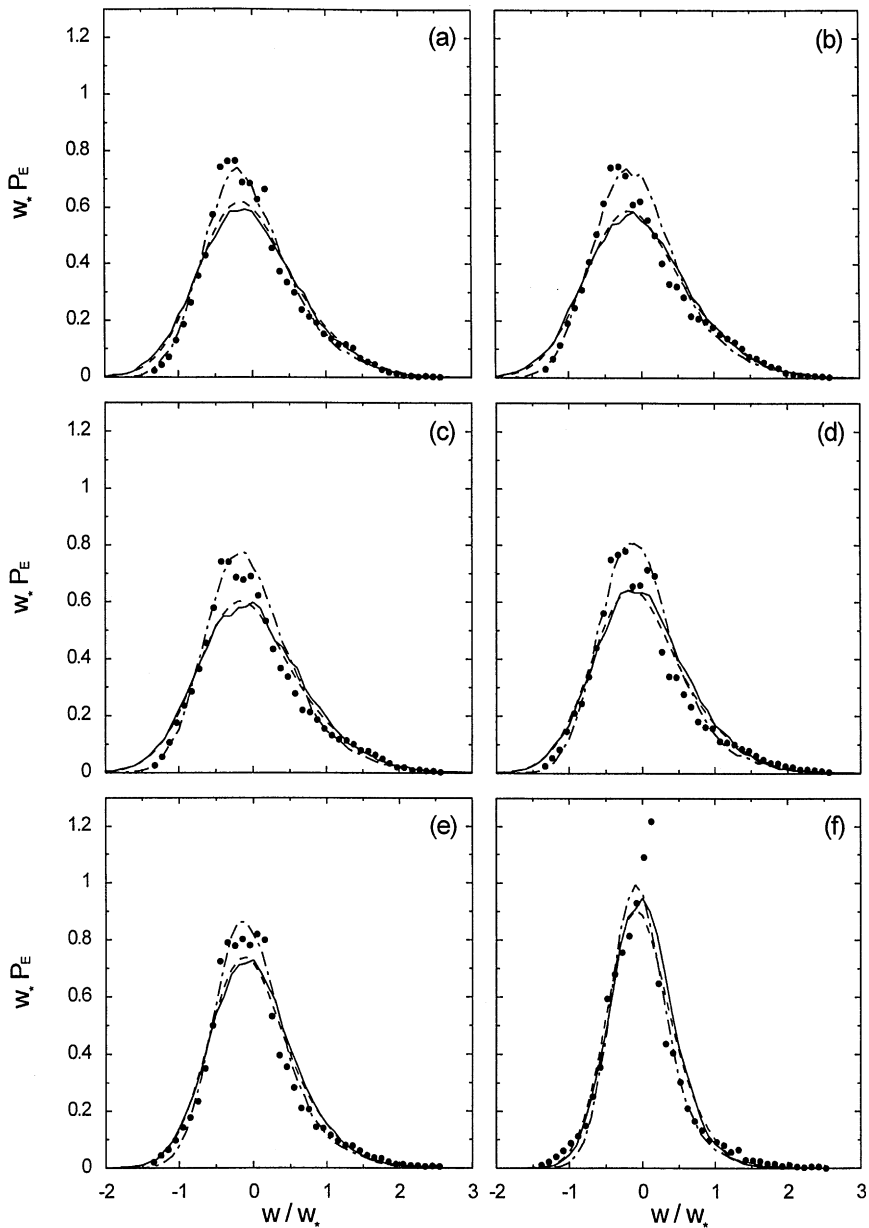


Fig. 9. Dimensionless vertical velocity probability density functions at heights (z/z_i) (a) 0.19, (b) 0.31, (c) 0.44, (d) 0.56, (e) 0.69 and (f) 0.81. Solid circles—water tank data (Luhar et al., 1996), solid line—new model results; dotted line—Luhar–Britter model results; dot–dash line—new model results for skewness $S = 0.75$ (second set of coefficients in Eqs. (7)).

probability distribution function of the velocity. The main strength of the model, however, lies in its simplicity and computational efficiency.

The dispersion results obtained from the new model were compared with existing laboratory data as well as with those obtained from a more complex Lagrangian model based on a bi-Gaussian velocity PDF. The comparison demonstrates that the new model performs well.

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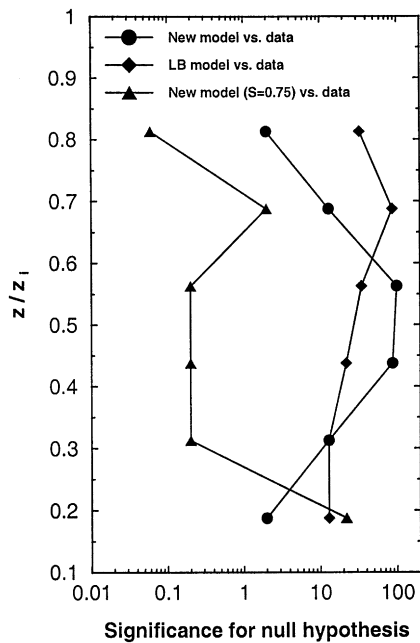


Fig. 10. Significance levels for the Kolmogorov–Smirnov statistics.

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