A two-dimensional Lagrangian stochastic dispersion model for daytime conditions

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(Received 9 February 1995; revised 13 July 1995)

Summary

A two-dimensional \((x, z)\) Lagrangian stochastic dispersion model is presented that is correct (i.e. fulfills the well-mixed condition) for neutral to convective conditions. The probability density function (pdf) of the particle velocities is constructed as a weighted sum of a neutral pdf \((u\) and \(w\) jointly Gaussian) and a convective pdf \((w\) skewed, \(u\) and \(w\) uncorrelated). The transition function \(\mathcal{F}\) varies continuously with stability and therefore ensures that the model results are not confined to a finite number of stability classes.

The model is described in full detail and some sensitivity tests are presented. In particular, the role of \(C_0\), the universal constant in the Lagrangian structure function for the inertial subrange, in determining average plume characteristics is discussed. Furthermore, the evolution of average plume-height and -width is investigated for different boundary-layer stabilities ranging from ideal neutral to fully convective. Finally, the model is applied to the situation of a tracer experiment in Copenhagen, and it is shown that the measured surface-concentrations can be well simulated.

Keywords: Boundary-layer stability Dispersion Particle model Plume characteristics

1. Introduction

Several different stochastic dispersion models have been presented in recent years to describe the dispersion of passive tracers in turbulent boundary layers. All have been shown to succeed in modelling the dispersion conditions in particular states of the boundary layer, such as inhomogeneous, skewed turbulence (e.g. Luhar and Britter 1989, hereafter referred to as LB89) or (inhomogeneous) Gaussian turbulence (e.g. Sawford and Guest 1988). In this study we present a two-dimensional approach which allows a continuous transition between Gaussian, correlated \((u, w)\) turbulence on the one hand, and skewed \((w)\), uncorrelated \((u, w)\) turbulence on the other; the latter is characteristic of convective boundary-layers. Thus the model may be applied in daytime conditions without requiring a decision on the choice of model.

Assuming the evolution of velocity \((u)\) and position \((x)\) of passive particles to be Markovian, the increments \(du_i\) and \(dx\) are most generally described by the stochastic differential equations (Thomson 1987, hereafter referred to as T87)

\[
\begin{align*}
    &du_i = a_i(x, u, t) \, dt + b_{ij}(x, u, t) \, d\xi_j \\
    &dx = u \, dt.
\end{align*}
\]

(1)

Here, the subscripts denote the velocity component under consideration \((i = 1, 3)\). The functions \(a_i\) may be viewed as the correlated part of the acceleration while the \(b_{ij}\) determine the random contribution, and \(d\xi\) must be the increment of a Wiener process with zero mean and variance \(dt\). T87 has analysed several selection criteria for models based on (1) and has shown that they are all equivalent or weaker than the well-mixed condition (which states, simply speaking, that particles initially well-mixed in position- and velocity-space remain well-mixed after a long application of the model). Based on this finding, he presented

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random-walk models for cases of three-dimensional (3-D) Gaussian or (weakly) skewed, one-dimensional (1-D) turbulence. LB89 derived a 1-D model that fulfils the well-mixed condition for the convective boundary-layer (CBL). Kaplan and Dinar (1993) used their so-called moments approximation to derive the model equations in three dimensions. In this approach there is no need for an a priori specification of the probability density function (pdf) of the particle velocities. However, it still requires an extra model formulation for each boundary-layer state. Furthermore, Du et al. (1994) have shown that a model based on this approximate solution of the Fokker–Planck equation is not well-mixed. Flesch and Wilson (1992) presented a two-dimensional (2-D) model that is based on Thomson’s criterion and is constructed from a pdf that is skewed in both \( u \) and \( w \). However, it does not have the correct (Gaussian) limit if either of the velocities (or both) actually has a Gaussian distribution; (see section 2(a)).

In the present paper, a 2-D \((u, w)\) model is presented that fulfils the well-mixed condition for any boundary-layer stability between neutral and fully convective. Clearly, this approach is more economical than a full 3-D model. It can still take the correlation between longitudinal and vertical velocity fluctuations into account, as this is very important near the ground where the turning of the wind vector with height is negligible. The model predicts crosswind integrated concentrations, which can be used to derive the crosswind distribution of concentration using a suitable model (Gryning et al. 1987). In the following, we recall the implications of the well-mixed condition for the design of a stochastic dispersion model (section 2), present an approach for generalized conditions of atmospheric turbulence that has very briefly been described by Rotach et al. (1994) (sections 3 and 4), investigate the properties and sensitivities of the model (section 5), and, finally, compare our results with measurements from a tracer experiment (section 6).

2. Model development

The well-mixed condition for the Markov process specified by (1) can be expressed by taking advantage of the fact that, under well-mixed conditions, the pdf of the particle velocities \( P_p \) is equal to that of the Eulerian velocities, here denoted as \( P_{tot} \). The Fokker–Planck equation for the process (1)

\[
\frac{\partial P_{tot}}{\partial t} = \frac{\partial}{\partial x_i}(u_i P_{tot}) - \frac{\partial}{\partial u_i}(a_i P_{tot}) + \frac{\partial^2}{\partial u_i \partial u_j} (B_{ij} P_{tot})
\]  

(2)

can then be used to derive the functions \( a_i \) and \( b_{ij} \). In (2) \( B_{ij} = \frac{1}{2} b_{ik} b_{jk} \), and the Einstein summation-convention applies. Following T87, (2) can be written for stationary turbulence

\[
a_i P_{tot} = \frac{\partial}{\partial u_j} (B_{ij} P_{tot}) + \Phi_i,
\]  

(3)

where \( \Phi \) obeys

\[
\frac{\partial \Phi_i}{\partial u_j} = - \frac{\partial}{\partial x_i}(u_i P_{tot}).
\]  

(4)

with the restriction on \( \Phi_i \) that \( \Phi_i \rightarrow 0 \) for \( |u| \rightarrow \infty \). From (4) it is apparent that, for descriptions of the flow in more than one dimension, the solution for \( \Phi \) is not unique: for every \( \Phi \) solving (4) there exists an infinite number of \( \Phi^* \), which are solenoidal in \( u \)-space (\( \partial \Phi^*/\partial u_i = 0 \)) so that \( \Phi + \Phi^* \) is also a solution to (4). Sawford and Guest (1988) examined this problem of non-uniqueness of the \( \Phi_i \)-functions by comparing two solutions for a simple flow. They show that the Lagrangian flow statistics are slightly different for the two solutions, thus indicating that an additional constraint is necessary to define a model uniquely. However, such a constraint has not yet been discovered (Sawford 1993).
2-D LAGRANGIAN STOCHASTIC DISPERSION MODEL

(a) The probability density function

The water-tank experiments of Willis and Deardorff (1976, 1978, 1981) and a first
generation of Lagrangian stochastic models (Lamb 1978) showed the importance of the
skewed pdf for vertical velocities when modelling dispersion in a CBL. Under conditions
of strong convection, the vertical and horizontal velocity fluctuations are only, at most,
weakly correlated and may therefore be assumed to be independent. On the other hand, with
decreasing instability, the pdf of the vertical velocity is observed to tend towards Gaussian
(Caughey et al. 1983). In the vicinity of the ground, where shear-produced turbulence
dominates, effects of correlation between horizontal and vertical velocity fluctuations
become important for the dispersion process (Legg 1983). These considerations lead to
the following construction of a 2-D total pdf $P_{tot}$:

*First limiting case: skewed in $w$, uncorrelated.* The pdf is described as $P_C P_u$, where
$P_u$ is a Gaussian distribution of the longitudinal velocity alone and $P_C$ is the skewed
vertical pdf as originally proposed by Baerentsen and Berkowitz (1984) and used in
the 1-D model of LB89:

$$P_C = A P_A + B P_B.$$  \hspace{2cm} (5)

$P_A$ and $P_B$ are both Gaussian and defined by

$$P_A = \frac{1}{\sqrt{2\pi}\sigma_A} \exp\left\{ -\frac{1}{2} \left( \frac{w - \bar{w}_A}{\sigma_A} \right)^2 \right\}, \quad P_B = \frac{1}{\sqrt{2\pi}\sigma_B} \exp\left\{ -\frac{1}{2} \left( \frac{w + \bar{w}_B}{\sigma_B} \right)^2 \right\}. \hspace{2cm} (6)$$

They refer to up- and down-draughts respectively. The parameters $A$ and $B$ may
be viewed as the (area) proportion of the CBL covered by up- and down-draughts.

*Second limiting case: correlated Gaussian.* As the other limiting case we consider
a purely Gaussian distribution

$$P_G = \frac{1}{(2\pi)^{3/2}(\det\mathbf{V})^{1/2}} \exp\left\{ -\frac{1}{2} \mathbf{u}^T \mathbf{V}^{-1} \mathbf{u} \right\} \hspace{2cm} (7)$$

where

$$\tilde{u}_i = u_i - \bar{u}_i, \quad \mathbf{V} = \begin{pmatrix} V_{11} & V_{12} \\ V_{12} & V_{22} \end{pmatrix}. \hspace{2cm} (8)$$

The subscript ‘G’ refers to ‘Gaussian’, $V_{ij}$ is the Gaussian covariance matrix, and
$\det\mathbf{V}$ its determinant. In two dimensions $P_G$ can be resolved into

$$P_G = P_u P_u P_{uw}. \hspace{2cm} (9)$$

Thus we have, using $(u, w)$ instead of $(u_1, u_3)$ for convenience and $\bar{w}_G = 0$:

$$P_u = \frac{1}{\sqrt{2\pi}\sigma_u} \exp\left\{ -\frac{1}{2} \frac{\tilde{u}_i^2}{(1 - \rho^2)\sigma_u^2} \right\}, \hspace{2cm} (10)$$

$$P_w = \frac{1}{\sqrt{2\pi}\sigma_w} \exp\left\{ -\frac{1}{2} \frac{w^2}{(1 - \rho^2)\sigma_w^2} \right\}, \hspace{2cm} (11)$$

and

$$P_{uw} = \frac{1}{\sqrt{2\pi}(1 - \rho^2)^{1/2}} \exp\left\{ \frac{\rho}{(1 - \rho^2)\sigma_u \sigma_w} \tilde{u} w \right\}. \hspace{2cm} (12)$$

where $\rho = \bar{u}\bar{w}_G / \sigma_u \sigma_w G$ is the correlation coefficient, and the elements of the co-
variance matrix are denoted as $V_{11} = \sigma_u^2$, $V_{22} = \sigma_w^2$ and $V_{12} = \bar{u}\bar{w}_G$. 
For the construction of the total 2-D pdf we first note the following property of $P_C$, the 1-D skewed distribution in $w$: constructing $a_w$ from $P_C$ (as done by LB89) leads to a form which does not relax—for $\overline{w^3} \to 0$—to the well-known expression

$$ a_w^{Gi} = -\frac{w}{\tau} + \frac{1}{2} \left( \frac{w^2}{\overline{w^2}} + 1 \right) \frac{\partial \overline{w^2}}{\partial z}, \quad (13) $$

which corresponds to the solution for a pdf describing Gaussian, inhomogeneous turbulence (Wilson et al. 1983; T87). This type of model will not, therefore, lead to a correct solution when approaching near-neutral conditions (for which the model of LB89 was never intended to be valid). Thus we construct a total 2-D pdf with the required asymptotic behaviour as follows:

$$ P_{\text{tot}} = \mathcal{F} P_C + (1 - \mathcal{F}) P_G = [\mathcal{F} P_C + (1 - \mathcal{F}) P_w P_{uw}] P_w \quad (14) $$

where $\mathcal{F}$ is a yet to be specified function of the height $z$, of the mixed layer height $z_i$ and of the Obukhov length $L$, describing a smooth transition between the two limiting cases. In (14), horizontal and vertical fluctuations are independent, and the distribution of the vertical velocity is skewed if $\mathcal{F} \neq 0$. On the other hand, if $\mathcal{F} = 0$, $\mathcal{F}$ and $w$ are jointly Gaussian distributed. When designing the function $\mathcal{F}$, the two limiting cases will be identified with a purely convective ($\mathcal{F} = 1$) and an ideally neutral boundary layer ($\mathcal{F} = 0$).

(b) Model functions $a_i$ and $b_{ij}$

The functions $b_{ij}$ in (1) can be specified using Kolmogorov's theory of local isotropy in the inertial subrange. Following T87, we have, if the frequency $dr^{-1}$, corresponding to the time-step, lies in the inertial subrange

$$ 2B_{ij} = \delta_{ij} C_0 \varepsilon. \quad (15) $$

$\varepsilon$ denotes the rate of dissipation of turbulent kinetic energy and $C_0$ a universal constant. There is some uncertainty concerning the value of $C_0$ (see Sawford and Guest 1988; Sawford 1993). The effect of varying the value of $C_0$ will be discussed in detail in section 5(b).

Using (15), and noting particularly that $B_{ij}$ was chosen to be independent of $u$, we can write the equation for the function $a_i$ from (3)

$$ a_i = \frac{1}{P_{\text{tot}}} (-B_* Q_i + \Phi_i), \quad (16) $$

where $B_* = B_{ii}$ and

$$ Q_i = -\frac{\partial P_{\text{tot}}}{\partial u_i}. \quad (17) $$

For the present pdf, the derivation of the $Q_i$ is straightforward

$$ Q_u = V_{11}^{-1} \overline{u} P_{\text{tot}} + (1 - \mathcal{F}) V_{12}^{-1} w P_G \quad (18) $$

$$ Q_w = \mathcal{F} Q_C P_w + (1 - \mathcal{F}) (V_{21}^{-1} w + V_{12}^{-1} \overline{u}) P_G, $$

where $Q_C$ is the one-dimensional solution arising from $P_C$ alone, and is given by LB89:

$$ Q_C = \frac{A(w - \overline{w}_A)}{\overline{w}_A^2} P_A + \frac{B(w + \overline{w}_B)}{\overline{w}_B^2} P_B. \quad (19) $$
To specify the functions $a_i$ fully, we have to derive expressions for the functions $\Phi_i$ that obey (4) with the restriction that $\Phi_i \to 0$ if $|u| \to \infty$. We consider here the stationary, horizontally homogeneous case with $P_{tot}$ as specified above. Derivation of the functions $\Phi_i$ is lengthy but straightforward and given in an appendix. We only note here that the $\Phi_i$ are formally split up into a Gaussian part $\Phi_i^G$ and a second contribution $\Phi_i^C$, reflecting the departure from the Gaussian solutions. Finally, to ensure that $\Phi_i \to 0$ if $|u| \to \infty$, an extra contribution $\Phi_i^*$ is introduced that is solenoidal in $u$-space and thus fulfills the requirement on $\Phi^*$ given above. Thus the solution reads

$$\Phi_i = \Phi_i^C + (1 - \mathcal{F}) \Phi_i^G + \Phi_i^*,$$  \hspace{1cm} (20)

where we use as a Gaussian solution the one given by T87; (see appendix for its explicit form). The two $\Phi_i^C$ are given by

$$\Phi_i^C = \frac{\partial \mathcal{F}}{\partial z} \frac{w}{2\sqrt{2\pi \sigma_{uG}}} \exp\{-\gamma w^2\} \text{erf}(\tilde{u}) + 1$$  \hspace{1cm} (21)

with the abbreviations

$$\gamma = \frac{2}{2\sigma_{uG}^2} > 0 \quad \text{and} \quad \tilde{u} = \frac{1}{\sqrt{2}} (V_{11}^{-1})^{1/2} \left[ u - \frac{\rho \sigma_{uG}}{\sigma_{uG}} w \right]$$  \hspace{1cm} (22)

and

$$\Phi_i^C = -(I_1 + I_2) \left[ \frac{\partial \mathcal{F}}{\partial z} P_u + \mathcal{F} \frac{\partial P_u}{\partial z} \right] + \mathcal{F} P_u \Phi_i^{1D},$$  \hspace{1cm} (23)

where $(I_1 + I_2) = \int_{-\infty}^{\infty} w P_C dw$ (following the notation of LB89) and $\Phi_i^{1D}$ is their 1-D solution for the vertical velocity. $\Phi_i^C$ goes to zero as $|u| \to \infty$ (see appendix). On the other hand, $\Phi_i^C$ only goes to zero for $|w| \to \infty$ and for $u \to -\infty$, but not so for $u \to +\infty$, where we obtain

$$\Phi_i^C(u = \infty) = \frac{\partial \mathcal{F}}{\partial z} \frac{w}{\sqrt{2\pi \sigma_{uG}}} \exp\{-\gamma w^2\}.$$  \hspace{1cm} (24)

Thus $\Phi_i^*$ is defined as

$$\Phi_i^* = -\frac{\partial \mathcal{F}}{\partial z} \frac{w}{2\sqrt{2\pi \sigma_{uG}}} \exp\{-\gamma w^2\} \text{erf}(\tilde{u}) + 1$$  \hspace{1cm} (25)

with the desired property that $\Phi_i^* \to 0$ as $u \to -\infty$ and $\Phi_i^* \to -\Phi_i^C$ for $u \to +\infty$. By defining furthermore

$$\Phi_i^* = -\frac{\partial \mathcal{F}}{\partial z} \frac{1}{(2)^{3/2} \pi \gamma \sigma_{uG}} \exp\{-\gamma w^2\} \exp\{-\tilde{u}^2\}$$  \hspace{1cm} (26)

it is easy to see that $\partial \Phi_i^*/\partial u_i = 0$.

(c) Normalization

The variables $\tilde{w}, \sigma_A, A, \tilde{w}_G, \sigma_B$ and $B$ and the parameters of the Gaussian distribution $\sigma_G, \sigma_{uG}$, $\tilde{w}_G$ and $\tilde{u}_G$ in $\Phi_i$ and $Q_i$ are determined by the requirement

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u^n w^m P_{tot}(u, w, z) \, du \, dw = \tilde{u}^n \tilde{w}^m(z),$$  \hspace{1cm} (27)
where $\bar{v}^w w^w(z)$ are the measured joint moments in the atmosphere. For $[n, m] = [1, 0]$, [1, 1] and [2, 0], the integration of (27) yields, respectively

$$\bar{u}_G = \bar{u}(z)$$  \hspace{1cm} (28)

$$\bar{u} \bar{w}_G = \frac{1}{1 - \mathcal{F}} \bar{u} \bar{w}(z)$$  \hspace{1cm} (29)

$$\sigma^2_{wG} = \bar{w}^2(z) + \frac{\bar{u} \bar{w}_G}{\sigma^2_{wG}} \mathcal{F}. $$  \hspace{1cm} (30)

Letting $n = 0$ and varying $m$ from 0 to 3 leads to a set of four equations for the remaining seven unknowns ($\sigma_{wG}$ and the variables in $P_G$). As an assumption to close the system, we use (LB89)

$$\bar{w}_A = \sigma_A, \quad \bar{w}_B = \sigma_B$$  \hspace{1cm} (31)

although the theoretical considerations of Hunt et al. (1988) indicate that the factor of proportionality between the mean velocities and standard deviations in $P_G$ is slightly different from one. The set of equations (27) with $n = 0, m = 0, 3$ can be solved with the closure (31) and an assumption for the vertical variance in $v_{G}, \sigma^2_{vG} = \bar{w}^2(z)$, to yield the following expressions for $A, \bar{w}_A, B$ and $\bar{w}_B$:

$$A + B = (1 - \rho^2)^{-1/2}$$  \hspace{1cm} (32)

$$\bar{w}_B = \frac{-w_A^2 + \sqrt{(w_A^2)^2 + 8\mathcal{F}^2(w_B^2)^3}}{4\mathcal{F}w^2}$$  \hspace{1cm} (33)

$$\bar{w}_A = \frac{w_A^2}{2\bar{w}_B}$$  \hspace{1cm} (34)

$$A = \frac{q \bar{w}_B}{w_A + \bar{w}_B}$$  \hspace{1cm} (35)

$$B = \frac{q \bar{w}_A}{w_A + \bar{w}_B}$$  \hspace{1cm} (36)

where we have used the abbreviation $q = (1 - \rho^2)^{-1/2}$.

In getting to expressions (33) to (36) we have used the restriction that $\mathcal{F} \neq 0$. However, if this is not the case, the four variables are not required to specify the total pdf; (see the definition of $P_{\text{tot}}$).

(d) Computational details

For each of the simulations presented in sections 5 and 6, a total number of 10,000 particles is released. At either boundary, $z = z_0$ and $z = z_i$, particles are fully elastically reflected; i.e. no absorption or transformation at the boundaries is taken into account. A number of authors have found that, in inhomogeneous turbulence, certain reflection conditions may lead to a violation of the well-mixed condition. Hurley and Physick (1993), for example, suggest changing a particle's vertical velocity upon reflection, so that a particle arriving at, say, the upper boundary with a velocity $w_{up}$ would be assigned a velocity $-cw_{up}$ after reflection, where $c$ is determined as the ratio of downdraught to updraught velocities ($c = \bar{w}_B / \bar{w}_A$). Thomson and Montgomery (1994) have shown that this reflection condition is not entirely able to fulfil the well-mixed condition if the velocity distribution is skewed at the boundaries. For our two-dimensional model, therefore, we follow the
recommendations of Wilson and Flesch (1993) and, at the reflecting boundary, change not only the vertical velocity to its negative counterpart, but also the horizontal (fluctuating) component. This ensures that the covariance also remains correct at the boundary and that the well-mixed condition can be met (Wilson and Flesch 1993). In the present model this reflection condition leads to a concentration profile that departs from the well-mixed value far downwind from the source (not shown) by less than 5%.

As a time-step criterion, an expression similar to that proposed by T87 is used:

$$\Delta t_{\text{max}} = \min \left( \frac{0.01 \sigma^2}{B}, \frac{0.1 \sigma}{|\sigma|}, \frac{0.01 \varepsilon}{|\mu \partial \sigma / \partial z|}, \frac{0.01 \varepsilon}{|\mu \partial \varepsilon / \partial z|} \right),$$  

(37)

where $\Delta t_{\text{max}}$ is the maximum allowed time-step. A default time-step $\Delta t$ is chosen for each model run. For the simulations of sections 5 and 6, $\Delta t = 0.1$ s. After the calculation of $ai$ and $bj$, (37) is evaluated for each particle separately. If, for a particle $i$, $\Delta t > \Delta t_{\text{max}}^i$, $\Delta t_{\text{max}}^i$ is used as a first step. Then a new position and new $ai$ and $bj$ are calculated (for this particular particle only) and $\Delta t_{\text{max}}^i$ is again determined. This procedure is repeated until the $\Delta t_{\text{max}}^i$ sum up to $\Delta t$ for particle $i$. With this procedure, we avoid prescribing a very small $\Delta t$ (in order to meet (37) at any possible position within the domain). Nevertheless, it is still relatively time-consuming as compared to ‘enforcing’ (37) by, for example, cutting the pdf at a certain threshold speed (LB89, as cited by Wilson and Flesch 1993). The only such commitment in the present model was to define the neutral contribution to the dissipation, $\varepsilon(z)$, that goes to infinity as $z \to 0$, in such a way that $\varepsilon(z < 5 \text{ m}) = \varepsilon(z = 5 \text{ m})$.

3. Parametrizations for Turbulence Statistics

If the atmospheric profiles of the velocity moments are not available, for example from a numerical model or observations, they may be parametrized. We consider here similarity formulations based on both mixed-layer scaling and observations in a neutral boundary layer to ensure a continuous transition according to stability.

For the profile of mean wind speed, Sorbian (1986) proposes

$$\frac{kz \partial \bar{u}}{u_* \partial z} = \Phi_m(z/L) \left( 1 - \alpha \frac{z}{z_i} \right)^{2/3},$$  

(38)

where $\Phi_m$ is the surface-layer expression for the non-dimensional wind-shear, $u_*$ the friction velocity, $k$ the von Kármán constant ($k = 0.4$) and $\alpha$ arises from $\theta(z) = \theta_0(1 - \alpha z/z_i)$. For $\Phi_m$ we use the formulation of Businger et al. (1971), modified after Höglström (1988). The choice for $\alpha$ gives some numerical problems. Batchvarova and Gryning (1990) suggest $\alpha = 1.2$, which leads to an undefined gradient of wind speed close to $z_i$. On the other hand, Stull (1988) suggests a formulation for the neutral boundary-layer that corresponds to $\alpha = 1.0$. During the present work, modelled profiles of $\bar{u}$ were calculated using $\alpha = 0$ and $\alpha = 1.2$, for both neutral and convective boundary layers. Only very small differences were found. Consequently, $\alpha = 1.0$ has been chosen for the present model.

The profile of Reynolds stress in a near-neutral boundary-layer has been parametrized by Brost et al. (1982) as

$$\bar{u} \bar{w}(z) = -u_*^2 \left( 1 - \frac{z}{z_i} \right).$$  

(39)

In order to obtain an expression for Reynolds stress that becomes approximately constant with height close to the surface (a region that was not covered by the measurements of
Brost et al. (1982), we use a slightly modified form for the profile of Reynolds stress, viz.

\[
\overline{uw}(z) = -u_i^2 \left( 1 - \exp \left( \frac{3(z - z_i)}{z_i} \right) \right).
\]

Identifying this neutral profile (40) with the Reynolds stress profile in the Gaussian pdf \( \overline{uw}_G \), we obtain from (29)

\[
\overline{uw}(z) = -u_i^2 (1 - \Psi) \left( 1 - \exp \left( \frac{3(z - z_i)}{z_i} \right) \right).
\]

Thus \( \overline{uw} \) is going to zero faster than linearly as height increases. This behaviour is often observed in CBLs (e.g. Kaimal et al. 1976; Chou et al. 1986).

The profile for the vertical velocity variances is adopted from Gryning et al. (1987):

\[
\frac{\overline{w^2}}{w_*^2} = 1.5 \left( \frac{z}{z_i} \right)^{2/3} \exp[-2(z/z_i)] + (1.7 - z/z_i) \left( \frac{w_*}{w_*} \right)^2.
\]

This expression is based on formulations for both neutral (Brost et al. 1982) and buoyancy-produced (Baerentsen and Berkowitz 1984) variance. The convective-velocity scale is defined as \( w_* = (g w^3 \theta(z)/\theta)^{1/3} \). For the longitudinal velocity variance, the starting point is an expression for \( \sigma_\varepsilon \) proposed by Gryning et al. (1987), but with the corresponding neutral formulation (Brost et al. 1982) for the longitudinal velocity variance

\[
\frac{\overline{u^2}}{u_*^2} = 0.35 \left( \frac{z}{z_i} \right)^{2/3} + \left( 5 - 4 \frac{z}{z_i} \right).
\]

The profile for the third moment of the vertical velocity is based on an expression given by Chou et al. (1986) for a CBL. The inclusion of data from other sources with different stabilities (Lenschow et al. 1980; Brost et al. 1982 and the water-tank data of Willis, cited by Baerentsen and Berkowitz (1984)) allows a re-evaluation of the (fitting) parameters in their formulation, yielding

\[
\frac{\overline{w^3}}{w_*^3} = 1.3 \left( \frac{z}{z_i} \right) \left( 1 - 0.8 \frac{z}{z_i} \right)^2.
\]

This parametrization, which fits the data reasonably well (Fig. 1), has the disadvantage that the skewness of the vertical-velocity distribution does not vanish at the top of the atmospheric boundary layer (ABL). Since the well-mixed condition cannot be fulfilled in this instance (see subsection 2(d)), we use, instead of (44),

\[
\frac{\overline{w^3}}{w_*^3} = 1.3 \left( \frac{z}{z_i} \right) \left( 1 - \frac{z}{z_i} \right)^2.
\]

Equation (45) underestimates the data in the upper part of the ABL (Fig. 1). However, as the most severely underestimated measurements are those from the near-neutral experiment (Brost et al. 1982), the chosen formulation seems justifiable.

Under convective conditions, the dissipation of turbulent kinetic energy \( \varepsilon \) can be described as follows (LB89)

\[
\frac{\varepsilon z_i}{w_*^3} = 1.5 - 1.2 \left( \frac{z}{z_i} \right)^{1/3}.
\]
Figure 1. The scaled third moment of the vertical velocity as a function of non-dimensional height. Data: + Brost et al. (1982), × Willis and Deardoff (personal communication cited by Baerentsen and Berkowitz 1984), * Chou et al. (1986), O Lenschow et al. (1980). The dashed line represents Eq. (44) and the solid line Eq. (45).

Figure 2. The near neutral profile for the normalized dissipation rate $\varepsilon$ according to Eq. (47), solid line, compared with measurements. Data: * Grant (1992), O Brost et al. (1982). The dashed line represents a surface layer parametrization after Vogel and Frenzen (1992).

For neutral stability on the other hand, a parametrization has been established using data from Brost et al. (1982) and Grant (1992)

$$\frac{\varepsilon z_i}{u^3} = a \frac{(1 - z/z_i)^2}{kz/z_i} + b,$$  \hspace{1cm} (47)

where the constants $a = 1.07$ and $b = 2.56$ are found from a parameter fit. Figure 2 shows that (47) represents the data reasonably well and that the parametrization is also suited to
describe the rate of dissipation within the surface layer; for this layer, a formulation after Vogel and Frenzen (1992) is plotted for comparison. Combining the two formulations (46) and (47) leads to a general description for the variation of $\varepsilon$ with height

$$
\varepsilon = \frac{u^3}{z_i} \left[ 1.07 \left( \frac{1 - z/z_i}{kz/z_i} \right)^2 + 2.56 \right] + \frac{w^3}{z} \left\{ 1.5 - 1.2 \left( \frac{z}{z_i} \right)^{1/3} \right\}.
$$

(48)

4. The transition function $\mathcal{F}$

From the definition of the total pdf $P_{tot}$, the function $\mathcal{F}$ approaches zero in purely Gaussian turbulence and unity in the case of a skewed velocity distribution in $w$ with vertical and horizontal fluctuations being independent. It is, therefore, one of the key features of the present model that the transition from a Gaussian to a skewed distribution in $w$, and from being correlated to being independent in $(u, w)$, is assumed to occur at the same rate (namely $\mathcal{F}$) as stability changes. This assumption has been made in order to keep the model as simple as possible and to avoid the introduction of two separate transition-functions. The most obvious approach to specifying the unknown $\mathcal{F}$ would be to include the fourth moment $\overline{w^4}$ into the normalization (Tassone et al. 1994). However, for the present 2-D pdf, it can be shown that this gives rise to unresolvable inconsistencies: (i) the $\mathcal{F}$-function obtained in this way leads to $\overline{u}$ and $w$ not being independent when values of $\mathcal{F}$ approach one (i.e. $\lim_{\mathcal{F} \to 1} \overline{a_u a_w} = \overline{a_u} \overline{a_w}$); and (ii) the parametrization of $\overline{w^4}$ has to fulfill certain constraints, which again make the model not universally applicable. These inconsistencies arise because, for simplicity, only one transition function has been introduced in $P_{tot}$. Consequently an attempt has been made to construct $\mathcal{F}$ from constraints on its behaviour in the two limiting cases as follows.

The function $\mathcal{F}$ has to be considered most generally as a function of $z$, $z_i$, and $L$. In order to obtain $\Phi_i = \Phi_i^G$ for $\mathcal{F} = 0$ and $\Phi_i = 0$ for $\mathcal{F} = 1$ (the accelerations in $u$ and $w$ then being independent) we have to require (from inspection of (21), (23), (25) and (26)) that the function $\mathcal{F}$ obeys

$$
\lim_{\mathcal{F} \to 0} \frac{\partial \mathcal{F}}{\partial z} = 0 \quad \text{and} \quad \lim_{\mathcal{F} \to 1} \frac{\partial \mathcal{F}}{\partial z} = 0.
$$

(49)

Furthermore, from (33) we see that the function $\mathcal{F}$ should approach zero more slowly than the third order moment $\overline{w^3}$, in order to remain well defined in the limit $\mathcal{F} \to 0$. Thus we have as a third model constraint

$$
\lim_{z/L \to 0} \frac{\overline{w^3}}{4 \mathcal{F}(w^2)} = 0.
$$

(50)

An obvious modelling assumption for $\mathcal{F}$ is to require that $\mathcal{F} \to 1$ in a fully convective boundary layer; i.e. if both $z/L$ and $z_i/L$ become large. It also seems to be convenient to let $\mathcal{F} \to 0$ in neutral stratification. However, this makes it impossible to fulfill the conditions (49) and (50) in the limit $z \to 0$ (unless the third order moment would also have a zero derivative as $z$ goes to zero; see (45)). Thus, we define $\mathcal{F}$ such that

$$
\lim_{z \to 0} \mathcal{F} = \delta \quad \text{and} \quad \lim_{u = 0} \mathcal{F} = 0;
$$

(51)

the latter condition refers to a boundary layer where turbulent heat flux is completely absent.
The simplest function that can be chosen is $\mathcal{F} = \mathcal{F}(z/L)$ alone (i.e. omitting the height dependence). This has the advantage of making the whole model much simpler, since all the $\partial \mathcal{F} / \partial z$-terms vanish; the price is that, in a convective boundary layer ($\mathcal{F} \approx 1$), the pdf for the vertical velocity fluctuations remains non-symmetric even in the surface layer, and that there is no correlation between $u$ and $w$.

A more general function that fulfils the above requirements is

$$\mathcal{F} = C_1 (C_2 - \cos g)$$

(52)

with

$$g = C_3 \pi (1 - \exp{z/L})$$

(53)

and $C_1$ and $C_2$ determined through equations (51) yielding

$$C_1 = \frac{1 - \delta}{2} \quad \text{and} \quad C_2 = \frac{1 + \delta}{1 - \delta}.$$  

(54)

From (51) we see that $\delta$ is zero if $w_*$ becomes zero. To make sure that $\delta$ is well-defined in the convective limit ($u_*$ going to zero), we use

$$\delta = \frac{\alpha_1 w_*}{u_* + \alpha_2}$$

(55)

where the values $\alpha_1 = 2.5 \times 10^{-2}$ m s$^{-1}$ and $\alpha_2 = 10^{-2}$ m s$^{-1}$ proved useful. Finally, the parameter $C_3$ is determined by fitting the pdf (14) with $\mathcal{F}$ described by (52) and (53) to experimental data from the literature (Godowitch 1986) and from an experiment on Anholt, a small island north-east of Denmark (Batchvarova and Gryning 1994). The best performance is obtained if $C_3$ is allowed to vary with stability, viz.

$$C_3 = 1 - C'_3 \left( \frac{u_*}{w_*} \right)^2$$

(56)

where $C'_3 = 1.65$. Note that in the neutral limit, where $C_3$ is not defined through (56), the function $g$ becomes zero and $C_3$ need not be specified. Figure 3 shows the height dependence of the function $\mathcal{F}$ for three different stabilities. Under near-neutral conditions, a large portion of the boundary layer is characterized by $\mathcal{F} \approx 0$, whereas in a highly convective boundary-layer $\mathcal{F} = 1$ (except in the first few metres above the ground).

5. MODEL VALIDATION AND SENSITIVITIES

(a) The probability density function

Since the starting point of the model is the construction of the 2-D velocity pdf, $P_{tot}$, we give some comparisons of the calculated and measured marginal probability density distribution, that is defined, for the vertical velocity for example, as

$$P_{\text{mar. } w} = \int_{-\infty}^{\infty} P_{\text{tot}} du = \mathcal{F}(1 - \rho^2)^{1/2} P_C + \left(1 - \mathcal{F} \right) \frac{1}{\sqrt{2\pi} \sigma_{wG}} \exp \left\{ -\frac{1}{2\sigma_{wG}^2} w^2 \right\}$$

(57)

and corresponds to the distribution in $w$ irrespective of the value of $u$. It is clear (and intended) from the construction of $P_{tot}$ that for $\mathcal{F} = 0$ the pdf becomes Gaussian—as observed, for example, by Caughey et al. (1983) in near-neutral conditions. In a CBL, on the other hand, $P_{\text{mar. } w}$ is—up to a factor $(1 - \rho^2)^{1/2}$—equal to the pdf given by LB89, who
showed that the water-tank results of Willis and Deardorff (1976, 1978, 1981) are well represented. These two limiting cases are not reproduced here. From Fig. 4 it becomes apparent that $P_{\text{tot}}$ is also suited to describe intermediate boundary-layer states. Having used the data shown in Fig. 4 to determine the parameter $C_3$ in the formulation of the transition function $\mathcal{F}$, this result is essentially a justification for the assumption that the turbulence characteristics change from Gaussian to skewed ($w$) and from correlated to independent ($u, w$) at approximately the same rate as stability increases.

(b) The universal constant $C_0$

A relatively wide range of values for the universal constant $C_0$ have been proposed
using different approaches:

— theoretical considerations yield \( C_0 = 7 \) (Sawford 1993; second-order autoregressive model) and \( C_0 = 5.7 \) (Rodean 1991; similarity arguments in the surface layer);

— the measurements of Hanna (1981) give \( C_0 = 4 \pm 2 \);

— a fit of modelled \( \sigma_z \) to wind-tunnel data indicates that the value of \( C_0 \) lies between 5 and 10 (Sawford and Geust 1988).

From these studies a value larger than 5 seems to be appropriate for \( C_0 \). Nevertheless, when modelling dispersion in a CBL, it is common to use \( C_0 = 2 \) (LB89; Hurley and Physick 1991, 1993; Physick et al. 1994; Tassone et al. 1994). The reason for this is apparent from Fig. 5. The ‘overshooting’ of both the average plume height \( \bar{z} / z_i \) and plume width \( \sigma_z / z_i \), as observed in the bench-mark water-tank experiments on convective dispersion characteristics by Willis and Deardorff (1976, 1978, 1981), can only be reproduced adequately when using a small value for \( C_0 \). Indeed, with the present model, the best representation of the water-tank data is found with \( 1.5 \leq C_0 \leq 2.5 \), the range arising for the three different initial heights in the experiments of Willis and Deardorff. As an example, in Fig. 6 the results for \( C_0 = 1.5, 2.0, 2.5 \) and 3.0 are shown along with the experimental data at an initial height \( z_{\text{init}} / z_i = 0.067 \) for comparison. Several other components of the model were also varied in attempts to have it reproduce the laboratory experiments of Willis and Deardorff (1976, 1978, 1981). These components included parametrizations of \( \overline{u^2} \) and \( \overline{w^3} \) (replacing the present parametrizations by those from LB89), the default time-step \( dz \), and also the time-step criterion (Eq. (37)). None of these changes resulted in more than a marginal difference in the dispersion characteristics. Furthermore, since it is always the product \( C_0 \varepsilon \) which appears, parametrization of \( \varepsilon \) was reconsidered. Equation (46), that is used in convective conditions, was originally suggested by LB89 and is based on data from the Minnesota and Ashchurch experiments. Caughey and Wyngaard (1979) mention that estimates of \( \varepsilon \) from the Minnesota experiment may be ‘erroneously high’ and dependent on boundary-layer stability, thus requiring a smaller value of \( C_0 \) to maintain the magnitude of the product \( C_0 \varepsilon \). However, the differences are far too small to explain the dependence of plume characteristics on \( C_0 \varepsilon \) as depicted in Fig. 5. Finally, the 1-D model of LB89 was
run with different values for $C_0$; (the water-tank experiments were essentially 1-D). The result is, as expected, very similar to the 2-D result of Fig. 5.

Thus, when fitting model results to the (convective) water-tank data, a small $\tilde{C}_0$ results, whereas a fit to the (neutral) wind-tunnel data (Sawford and Guest 1988) suggests a much larger value, similar to the theoretical estimates. Similarly, Rotach (1995a) compares the ideally neutral results of a large eddy simulation (LES) by Mason (1992) with those of the present model and concludes that, in contrast to the present findings for a CBL, a value of at least $C_0 = 7$ is necessary to match the LES plume characteristics. Sawford (1991, 1993) points out that care must be taken when fitting model predictions to laboratory data or results of direct numerical simulations obtained at low Reynolds numbers, in order to estimate a numerical value for $C_0$. Then, due to Reynolds-number effects, a value $C_0^*$ is found rather than $C_0$, the universal constant in the infinite Reynolds-number limit. The two constants are related through

$$C_0^* = C_0(1 + Re_s^{-1/2})^{-1} \quad (58)$$

where $Re_s$, the Lagrangian Reynolds-number, is defined as

$$Re_s = \left( \frac{16 a_0^2 t_E^2}{C_0^4 t_K^2} \right) \quad (59)$$

and $t_K = (\nu/\varepsilon)^{1/2}$ is the Kolmogorov microscale and $t_E = \sigma^2/\varepsilon$ the timescale corresponding to the energy-containing scales of turbulence. Here, $a_0$ is another universal constant (in the limit of large Reynolds-numbers) associated with the magnitude of the acceleration variance (Sawford 1993). For the water-tank experiments, $Re_s$ can be estimated at 6.4–8.5 (the range again arising for the three initial heights) using the expression of Sawford (1991) for the Reynolds-number dependence of $a_0$. Hence, using (58), the ratio $C_0/C_0^*$ is found to lie between 1.3 and 1.4 and our fit to the water-tank data finally yields an optimal value for $C_0$ in the range 2.1–3.4. The same exercise carried out on the wind-tunnel data of Legg (1983), which were used by Sawford and Guest (1988), gives a value of $C_{w}/C_0^*$ very close to unity.
From these considerations we conclude that there is still considerable uncertainty about the correct numerical value of the constant $C_0$ to be used in stochastic particle models. Even when considering Reynolds-number effects, a fit to the water-tank data gives a value for $C_0$ that is a factor of two or so smaller than the theoretical predictions cited above. On the other hand, the characteristic overshooting of the average plume height and plume spread cannot be reproduced unless a relatively small value is used. Bearing in mind that this overshooting is also observed in atmospheric dispersion experiments (Briggs 1993), it is concluded that the value of approximately three found above is appropriate for atmospheric applications, at least under convective conditions. So, henceforward, $C_0 = 3$ is used for all boundary-layer stabilities.

\( (c) \quad \text{Stability} \)

Five characteristic boundary-layer states are now investigated, using the scaling parameters listed in Table 1. Stability varies from purely convective (case A) to ideally neutral (case E). Cases B and D represent non-ideally convective and neutral situations respectively, and case C is at intermediate stability. The profiles of $\mathcal{F}$ for cases B, C and D are presented in Fig. 3.

Under convective conditions, concentration characteristics can universally be described as a function of a non-dimensional time $T_* = t w_*/z_i$. Since we are interested in stability ranging from convective to neutral, $T_*$ is not particularly useful. Thus we used the mixed velocity scale proposed by Troen and Mahrt (1986). For momentum, $w_m$ is defined here using the expression of Troen and Mahrt for the outer layer

\[
    w_m = (u^*_e + \beta_1 w^*_e)^{1/3},
\]

where $\beta_1 = 0.6$ (Holtslag and Boville 1993). For heat and moisture, $w_i$ is defined for the outer layer according to

\[
    w_i = \frac{w_m}{Pr},
\]

where $Pr$ is the Prandtl number

\[
    Pr = \frac{\phi_h(z/L)}{\phi_m(z/L)} + \beta_2 \frac{k}{h} \frac{z}{w_m}.
\]

$\phi_h$ is the non-dimensional temperature gradient and $\beta_2 = 7.2$ (Holtslag and Boville 1993). To calculate $w_i$ in the outer layer, $Pr$ is evaluated at the top of the surface layer (i.e. at $z/z_i = 0.1$). In Figs. 7 and 8, $\vec{z}/z_i$ and $\sigma_z/z_i$ for the five cases (Table 1) and a source height of $z_{m}/z_i = 0.115$ are plotted against non-dimensional time, calculated either using $w_i (T_{i} = t w_i/z_i; \text{Fig. 7})$ or $w_m (T_{m} = t w_m/z_i; \text{Fig. 8})$. Although it is often argued that passive tracers disperse and mix like heat and moisture, $w_m$ is apparently better suited to

<table>
<thead>
<tr>
<th>Case</th>
<th>$u^*_e$ (m s$^{-1}$)</th>
<th>$w^*_e$ (m s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.6</td>
<td>2.0</td>
</tr>
<tr>
<td>B</td>
<td>0.3</td>
<td>2.0</td>
</tr>
<tr>
<td>C</td>
<td>0.4</td>
<td>1.0</td>
</tr>
<tr>
<td>D</td>
<td>0.8</td>
<td>0.5</td>
</tr>
<tr>
<td>E</td>
<td>0.7</td>
<td>0.0</td>
</tr>
</tbody>
</table>
describe the temporal evolution of the plumes for a wide range of boundary-layer stabilities than is \( u_0 \). In the non-neutral cases the maximum of the scaled average plume-height, as well as the plume-width, is reached at \( T_{sm} \) between 1.5 and 2.0. At \( T_{sm} > 3 \) the equilibrium values \( \bar{z}/z_i = 0.5 \) and \( \sigma_z/z_i = (\int_0^\infty (Z - Z_{ini})^2 dZ)^{1/2} \), \( Z = z/z_i \) are approached. For the two (near-) neutral cases D and E the equilibrium values are approached without going through a maximum at \( T_{sm} \approx 2 \). If plotted against \( T_{sm} \), the five cases still exhibit considerably different values of the maxima or minima in \( \bar{z}/z_i \) or \( \sigma_z/z_i \). This is shown in more detail in Fig. 9, where the five cases are plotted for an initial height \( z_{ini}/z_i = 0.49 \). As a result of the skewed vertical-velocity distribution, the average plume initially descends to about \( \bar{z}/z_i = 0.42 \) in the convective cases A and B, whereas in the (near-) neutral cases D and E only a minor 'dip' is observed. For this height of emission, the equilibrium plume-height and -width are reached by \( T_{sm} \approx 1 \).
The present results can be compared with those of Mason (1992), who uses LES to assess the dispersion characteristics under varying stability. The present cases A, C, D and E correspond best to Mason's runs R0, R7, R10 and R20N respectively. His non-dimensional source-height ranges from 0.09 to 0.13. For comparison, the present \( \bar{z}/z_i \) and \( \sigma_z/z_i \) for the emission height \( z_{em}/z_i = 0.115 \) are plotted as a function of time in Fig. 10. A good overall qualitative correspondence between the present results and those obtained by Mason can be observed. The increase of \( \bar{z}/z_i \) and \( \sigma_z/z_i \) is much faster in convective conditions than in the near-neutral cases. The most important difference again lies in the ideally neutral run (R20N of Mason and the present case E). Whereas, in the LES, neither \( \bar{z}/z_i \) nor \( \sigma_z/z_i \) reaches its equilibrium value after 4000 s of simulation, Fig. 10 shows that with the present model the average plume-height and plume-width are reached after slightly more than 3000 s. It is noteworthy that the correspondence is much better for the two near-neutral simulations (Mason's R10 and the present case D).
Since Mason (1992) is modelling the turbulence structure of the boundary layer in much more detail than the present authors, this comparison gives us confidence that the chosen model approach and, in particular, the construction of the velocity pdf according to (14) leads to a realistic description of turbulence and hence diffusion for boundary-layer stabilities between ideally neutral and fully convective.

6. Comparison with field data

In a tracer experiment, SF₆ was released at a height of 115 m over the city of Copenhagen during periods lasting approximately one hour (Gryning and Lyck 1984). Surface measurements were taken on two or three arcs at distances of roughly 2, 4 and 6 km from the source. Each arc consisted of about 20 samplers and allowed the determination of a cross-wind integrated ground-level concentration (GLC) $ar{C}_i$. Ten experiments were performed in total, with stabilities ranging from mixed convective ($u_* = 2.1$ m s⁻¹, $u_* = 0.7$ m s⁻¹) to near-neutral ($u_* = 0.7$ m s⁻¹, $u_* = 0.4$ m s⁻¹). At the source height, measurements are available of $u_*$, of the vertical velocity variance and of the mean wind speed as well as standard meteorological profiles of wind speed and temperature up to a height of 200 m. The depth of the mixed layer was determined from radio soundings and varied between roughly one and two kilometres, so that the non-dimensional release height was $z_{mi}/z_0 \approx 0.05–0.1$. The roughness length was estimated at 0.6 m. The area over which the experiments were performed is suburban residential with a fairly homogeneous distribution of roughness elements (buildings, vegetation). At some distance from the surface the conditions for dispersion can be considered horizontally homogeneous. The experiments represent one of the reference datasets for a European effort to harmonize short-range dispersion models (Ølesen and Mikkelsen 1992).

The parametrized vertical velocity variance overestimates the measurements at 115 m by, typically, 30%. Therefore, the profile of the second moment of the vertical velocity is multiplied by $w_{\text{meas}}^2 / w_{\text{pas}}^2$ at 115 m (or this ratio’s 3/2 power for $w^3$) in order to match the observations at the source height (Tassone et al. 1994). (In one of the experiments, this ratio becomes larger than four, and this experiment is omitted from the analysis.) Similarly, the profile of mean wind speed is shifted in such a way, that the measurements at 10 m and 115 m above ground are optimally reproduced. Surface concentrations are determined by counting particles in boxes of dimensions $dz \approx 20$ m and $dx \approx 300$ m.

In Fig. 11, the measured and modelled cross-wind integrated GLCs for the Copenhagen tracer experiment are compared. The correspondence can be considered good, with an r.m.s. difference between measured and modelled concentrations of 0.46 mg m⁻² and an average measured concentration of 1.43 mg m⁻². On average, the relative difference between model estimates and observations is 24%. The model underestimated the GLC (average fractional bias 0.21), this being most pronounced for those experiments in which relatively high concentrations were observed far downwind from the source. In Fig. 12 the simulation of the experiment of 19 October 1978 is depicted. The model results show that the position of the maximum GLC was (presumably) not captured by the measurements and, furthermore, that modelled values of the concentration farther downwind from the source decreased more rapidly than measured values. Rotach (1995b) investigates the influence on dispersion of a roughness sub-layer. For a source close to such a rough surface, the position of the maximum GLC is found to be slightly farther downwind (some tens of metres) in the ‘rough wall’ simulation and the concentration to decrease more slowly in the lee of the maximum. Since the Copenhagen experiments were performed over a rather rough surface, this is in line with the tendency of the present model to underestimate the GLC.
Figure 11. Modelled versus measured cross-wind integrated ground level concentrations for the tracer experiments in Copenhagen (measurements from Gryning and Lyck 1984).

Figure 12. The cross-wind integrated ground level concentration $\bar{C}_y$ as a function of distance from the source for the tracer experiment of 19 October 1978 in Copenhagen. The solid line denotes the model simulation and the crosses the measurements (Gryning and Lyck 1984).

Similar results have been presented by Tassone et al. (1994), who used a 1-D stochastic dispersion model that also allowed for varying boundary-layer stability. Their results again show a tendency of the simulations to underestimate the measurements, along with a larger r.m.s. difference between observations and model estimates than in the present simulations. This indicates that the introduction of horizontal velocity fluctuations improves the overall model performance. Nevertheless, it is clear that for a source height of 115 m, the short-time dispersion takes place at a height where the correlation of the velocity components is probably of minor importance.

7. Summary and Conclusions

A 2-D Lagrangian stochastic particle-dispersion model is presented that fulfils the well-mixed condition after Thomson (1987). It is designed to be correct for any stability between ideally neutral and fully convective and therefore allows for modelling dispersion
in a continuously-evolving daytime boundary-layer without assigning stability classes or ‘switching’ from one model to another as stability changes. An extension of the approach to stable stratification is straightforward and requires only an investigation of velocity pdf’s under stable conditions. The model realistically reproduces measured velocity pdf’s as well as dispersion characteristics obtained from (i) the Willis and Deardorff water-tank experiments, (ii) large eddy simulations and (iii) a full-scale tracer experiment; it is concluded that the chosen approach incorporates the essential processes of daytime dispersion. Analysis of the results from the tracer experiment indicates, furthermore, that the introduction of correlations between longitudinal and vertical velocities (in contrast to taking only the vertical velocity fluctuations into account) leads to a better correspondence with the measurements.

The model is used to investigate the value of \( C_0 \), the universal constant in the inertial subrange form for the Lagrangian structure function. It is shown that with a value larger than 5 for \( C_0 \), as suggested by theoretical studies, the ‘overshooting’ of both the average plume height and width, as observed by Willis and Deardorff in convective water-tank experiments, cannot be reproduced. From a detailed investigation of the model performance, taking the small Reynolds-number of the water-tank experiments into account, it is concluded that \( C_0 \approx 3 \) may be appropriate for modelling dispersion in convective atmospheric boundary layers.

From a series of experiments with varying boundary-layer stability, the dispersion characteristics from releases near ground level are found to be well described when expressed as a function of \( T_{\ast m} = tw_m / z_\ast \), where \( w_m \) is a mixed velocity scale for momentum.

**ACKNOWLEDGEMENTS**

This project was supported by the Swiss National Science Foundation, the Swiss Federal Institute of Technology (MWR) and by the Commission of the European Community under the STEP program (CT).

**APPENDIX**

**Derivation of the functions \( \Phi \)**

The functions \( \Phi \) are determined by (4) which, in the case of stationary, horizontally homogeneous turbulence and with \( P_{\text{tot}} \) defined by (14), is given by

\[
\frac{\partial \Phi_u}{\partial u} + \frac{\partial \Phi_w}{\partial w} = -\frac{\partial}{\partial z}(w P_C P_u) - \frac{\partial}{\partial z}[(1 - \bar{\Phi}) w P_G].
\]  
(A.1)

In particular, we note from (A.1) that in the two- (or more) dimensional case, the solution is not unique: for \( (\Phi_u, \Phi_w) \) solving (A.1) any \( (\Phi^*_u, \Phi^*_w) \) can be added if

\[
\frac{\partial \Phi^*_u}{\partial u} + \frac{\partial \Phi^*_w}{\partial w} = 0.
\]  
(A.2)

thus leading to an infinite number of solutions.

We split \( \Phi \) into \( \Phi = \Phi^1 + \Phi^C \) and equate \( \Phi^C \) with the first term on the right-hand side of (A.1)

\[
\frac{\partial \Phi^C}{\partial w} = -\frac{\partial}{\partial z}(w P_C P_u) - \frac{\partial}{\partial z} P_C - \bar{\Phi} w P_C \frac{\partial P_u}{\partial z}.
\]  
(A.3)
Integrating (A.3) yields
\[ \Phi^c_w = -\frac{\partial F}{\partial z} P_u \int_{-\infty}^{w} w' P_c dw' - F P_u \int_{-\infty}^{w} w' \frac{\partial P_c}{\partial z} dw' - F \frac{\partial P_u}{\partial z} \int_{-\infty}^{w} w' P_c dw' \]  
(A.4)
and can be rewritten to yield (23) by identifying the integral in the second term on the right-hand side of (A.4) as the 1-D solution of LB89, \( \Phi^D_w \), and using their notation for \( \int_{-\infty}^{w} w' P_c dw' = I_1 + I_2 \). It is easy to see that \( \Phi^c_w \) goes to zero as \( |u| \to \infty \) (since \( P_u \) goes to zero) or \( |w| \to \infty \) (by noting that \( (I_1 + I_2) \to 0 \), and \( \Phi^D_w \to 0 \)).

Now, subtracting (A.3) from (A.1), we are left with
\[ \frac{\partial \Phi_u}{\partial u} + \frac{\partial \Phi^1_w}{\partial w} = -(1 - F) \frac{\partial}{\partial z} (w P_G) + w P_G \frac{\partial F}{\partial z}. \]
(A.5)
We denote a Gaussian solution to an equation of the form (4) as \( (\Phi^G_u, \Phi^G_w) \):
\[ \frac{\partial \Phi^G_u}{\partial u} + \frac{\partial \Phi^G_w}{\partial w} = -\frac{\partial}{\partial z} (w P_G) \]
(in the special case that \( \partial/\partial x = \partial/\partial t = 0 \)) and note that
\[ (1 - F) \left( \frac{\partial \Phi^G_u}{\partial u} + \frac{\partial \Phi^G_w}{\partial w} \right) = -(1 - F) \frac{\partial}{\partial z} (w P_G). \]
(A.7)
Thus we can further split up the \( \Phi_i \) according to \( \Phi_u = \Phi^C_u + (1 - F) \Phi^G_u \) and \( \Phi_w = \Phi^C_w + (1 - F) \Phi^G_w + \Phi^G_w \). Since \( F \) is independent of \( u \) and \( w \), we can subtract (A.7) from (A.5), thus leaving
\[ \frac{\partial \Phi^C_u}{\partial u} + \frac{\partial \Phi^C_w}{\partial w} = w P_G \frac{\partial F}{\partial z}. \]
(A.8)
We set \( \Phi^C_u = 0 \) and integrate (A.8) to yield (21) for \( \Phi^C_u \). Due to \( \nu \geq 0 \) (Eq. (22)) we have \( \Phi^C_u \to 0 \) as \( |w| \to \infty \) and since \( \text{erf}(-\infty) = -1 \) also for \( u \to -\infty \). On the other hand, for \( u \to +\infty \) we have \( \Phi^C_u(u = \infty) \neq 0 \) (Eq. (24)). We therefore make use of (A.2) and define \( \Phi^*_u \) as in (25) with the required property that \( \Phi^* \rightarrow 0 \) as \( u \to -\infty \) and \( \Phi^*_u \rightarrow -\Phi^C_u \) for \( u \to +\infty \). As outlined in subsection 2(b), \( \Phi^*_u \) may then be defined according to (26); (A.2) is met, as can easily be seen by differentiating (25) and (26).

The final solution now reads
\[ \Phi_i = \Phi^C_i + (1 - F) \Phi^G_i + \Phi^*_i, \]
(A.9)
where we use for the Gaussian part of the solution the one given by T87, which, in the present notation, is given by
\[ \frac{\Phi^C_w}{P_G} = \frac{1}{2} \left\{ \left( V_{11}^{-1} \frac{\partial V_{11}}{\partial z} + V_{12}^{-1} \frac{\partial V_{12}}{\partial z} \right) \tilde{u} w + \left( V_{12}^{-1} \frac{\partial V_{11}}{\partial z} + V_{22}^{-1} \frac{\partial V_{12}}{\partial z} \right) w^2 \quad \right. \\
+ \left. 2 \frac{\partial \tilde{u}}{\partial z} w + \frac{\partial V_{12}}{\partial z} \right\} 
\]
(A.10)
\[ \frac{\Phi^C_w}{P_G} = \frac{1}{2} \left\{ \left( V_{11}^{-1} \frac{\partial V_{12}}{\partial z} + V_{12}^{-1} \frac{\partial V_{22}}{\partial z} \right) \tilde{u} w + \left( V_{12}^{-1} \frac{\partial V_{12}}{\partial z} + V_{22}^{-1} \frac{\partial V_{22}}{\partial z} \right) w^2 + \frac{\partial V_{22}}{\partial z} \right\}. 
\]
(A.11)
Thus, through (20), together with (21), (23), (25), (26), (A.10) and (A.11), the two functions \( \Phi_u \) and \( \Phi_w \) are completely specified.
REFERENCES


2-D LAGRANGIAN STOCHASTIC DISPERSION MODEL


