Dispersion of a Passive Tracer in Buoyancy- and Shear-Driven Boundary Layers

ALESSANDRO DOSIO, JORDI VILA-GUERAU DE ARELLANO, AND ALBERT A. M. HOLTSLAG

Meteorology and Air Quality Section, Wageningen University, Wageningen, Netherlands

PETER J. H. BUILTJES

TNO-MEP, Apeldoorn, Netherlands

(Manuscript received 4 November 2002, in final form 20 February 2003)

ABSTRACT

By means of finescale modeling [large-eddy simulation (LES)], the combined effect of thermal and mechanical forcing on the dispersion of a plume in a convective boundary layer is investigated. Dispersion of a passive tracer is studied in various atmospheric turbulent flows, from pure convective to almost neutral, classified according to the scaling parameters $u^*/w^*$ and $z_i/L$. The LES results for the flow statistics and dispersion characteristics are first validated for pure convective cases against the available results from laboratory and field experiments. Currently used parameterizations are evaluated with the model results. The effect of wind shear is studied by analyzing the dynamic variables, in particular the velocity variances, and their relation with the dispersion characteristics, specifically plume mean height, dispersion parameters, ground concentrations, and concentration fluctuations. The main effect of the wind shear results in a reduction of the vertical spread and an enhancement of the horizontal dispersion. This effect greatly influences the behavior of the ground concentrations because the tracer is transported by the wind for a longer time before reaching the ground. The vertical dispersion parameter is studied by discussing the two main components: meandering and relative diffusion. Results show that the increasing wind reduces the plume vertical motion. The influence of increasing wind shear on the concentration fluctuation intensity is also analyzed. The limited plume vertical loopin in conditions of weak convection results in a reduction of the concentration fluctuation intensity. Parameterizations for the dispersion parameters are derived as a function of the flow characteristics, namely, the shear–buoyancy ratio, velocity variances, and wind shear. The parameterizations are partially based on previous studies and are verified for the different buoyancy- and shear-driven flows, showing satisfactory agreement with the model results.

1. Introduction

Atmospheric dispersion is a process governed by the turbulent characteristics of the atmospheric boundary layer (ABL). The structure of the ABL during convective conditions [convective boundary layer, hereinafter (CBL)] is strongly influenced by the combination of the thermal (buoyancy) and mechanical (wind shear) forcing. In very unstable conditions ($-z_i/L > 10$, where $z_i$ is the height of the CBL and $L$ is the Monin–Obukhov length), buoyancy is the main driving mechanism for the turbulence production through the whole layer, and the flow field is characterized by large subsidence motions of cold air (downdrafts) surrounded by narrow strong updrafts of warm air. The effect of this asymmetric turbulent structure on dispersion was widely investigated by means of laboratory experiments (Willis and Deardorff 1976, 1981; Deardorff and Willis 1985; Weil et al. 2002), field campaigns (Briggs 1993), and numerical simulations using finescale models that resolved explicitly the most relevant scales of the CBL (Lamb 1982; Heny and Sykes 1992; Nieuwstadt and de Valk 1987; Nieuwstadt 1992; Liu and Leung 2001).

In contrast with this flow, the structure of the CBL in conditions of weaker stability ($-z_i/L < 10$), when the flow is forced by the combined effect of buoyancy and shear, was studied recently, and the formation of two-dimensional roll structures aligned with the wind was observed. The turbulent field was classified according to scaling parameters such as the shear–buoyancy ratio $u^*/w^*$ (where $u^*$ is the friction velocity and $w^*$ is the convective velocity scale) and it was found to be different from either the pure convective or pure shear flow, as shown, for example, by Moeng and Sullivan (1994) and Sykes and Heny (1989). Here, $g$ is the acceleration of gravity, $\theta$ is potential temperature, $w$ is vertical velocity, primes indicate perturbations, and an overbar indicates averaging.

However, less is known about the dispersion in this situation of weak and moderate convection ($-z_i/L < 10$).
10) as pointed out by Weil (1988). Only a few studies (Mason 1992; Gopalakrishnan and Avisar 2000; Luahr 2002; Fedorovich and Thäter 2002) have investigated dispersion in a CBL driven by both shear and buoyancy. In those works, results from (mainly) stochastic models and wind tunnel experiments were presented, and only Mason (1992) used a large-eddy simulation (LES) model to investigate the evolution of the dispersion parameters. In his study, however, a clear systematic relationship between the properties of the turbulent flow and the dispersion characteristics under various stability regimes was missing.

Here we use an LES to generate CBLs with different combinations of surface heat flux and geostrophic wind. The simulated CBLs range from pure convective to near-neutral conditions, and they are classified according to scaling parameters such as \( u_*/w_a \) and \(-z_i/L\). The dispersion characteristics of a plume of passive scalar released at different heights are studied as a function of these dimensionless parameters. In addition, the effect of the increasing wind shear on the plume meandering and the concentration fluctuations is discussed in relation to the different stability regimes.

Once the dispersion process is described in terms of the scaling parameters, we propose parameterizations for the dispersion parameters \( \sigma_u \) and \( \sigma_w \) for flows driven by the combined effect of buoyancy and shear. In conditions of weak convection, in fact, the understanding of the dispersion process still presents large uncertainties (Weil 1988), and suitable parameterizations of the dispersion parameters are therefore needed.

In section 2 we describe the numerical code used and the classification of the various simulated CBLs. The LES results for the flow structure and dispersion characteristics are thoroughly discussed in section 3, where they are validated for the pure convective cases, for which extensive datasets are available. The effect of increasing wind shear on the flow dynamics (velocity variances) and dispersion statistics is then studied in section 4. The parameterization for the dispersion parameters in buoyancy- and shear-driven boundary layers (BLs) are proposed in section 5 and are validated against the LES results. Symbols are listed and defined in an appendix.

2. Description of the numerical experiment

The LES code used in this work is described by Cuypers and Duynkerke (1993) and Siebesma and Cuypers (1995), in which a set of filtered prognostic equations for the dynamic variables (wind velocity, potential temperature, and turbulent kinetic energy) is solved on a staggered numerical grid. The subgrid fluxes are closed by relating them to the gradient of the solved variable by means of an exchange coefficient. A conservation equation for the passive tracer is added to the governing set of equations. It reads

\[
\frac{\partial \bar{\psi}}{\partial t} = -\bar{u}_i \frac{\partial \bar{\psi}}{\partial x_i} - \bar{u}_i' \bar{\psi}'^*,
\]

where \( \bar{\psi} \) is the mean (filtered) scalar concentration, \( \bar{u}_i \) is the mean wind, and \( \bar{u}_i' \bar{\psi}'^* \) is the subgrid flux. The space and time integrations are computed with a kappa (Vreugdenhil and Koren 1993) and a Runge–Kutta numerical scheme, respectively. Lateral periodic boundary conditions are imposed for all the variables. However, as soon as the scalar reaches the lateral boundaries the simulation is ended, because the plume statistics become meaningless. A time step of 1 s is used.

Four different values of the geostrophic wind (0.5, 10, 15 m s\(^{-1}\)) and three different surface heat fluxes (0.052, 0.1, 0.156 K m s\(^{-1}\)) are prescribed in order to generate CBLs with different combinations of thermal and mechanical forcing.

The numerical domain covers an area of 10 km \( \times \) 10 km, solved with a horizontal grid length of 62.5 m. A grid of 40 points is used in the vertical direction; the vertical grid spacing (25, 30, and 50 m) is modified, depending on the case being investigated, on the basis of the different initial conditions (surface heat flux). The CBL height is computed by analyzing the vertical profile of a constant surface flux. The value of the roughness length \( z_0 \) is set to 0.15 m for all of the cases.

The aspect ratio, that is, the ratio between the horizontal domain dimension and the CBL height, varies from 6.6 for the most convective case \((z_0 \sim 1500 \text{ m})\) to 12 for the near-neutral one \((z_0 \sim 800 \text{ m})\).

An initialization period (i.e., the period of CBL development) of 4 h is needed to ensure that a (quasi) stationary state is reached for all of the simulated flows. The simulated wind profiles are characterized by shear at the bottom and at the top of the BL. Moreover, for high values of the geostrophic wind, a change of the wind direction with height is observed.

The simulated CBLs are classified according to the values of the shear–buoyancy ratio \( u_*/w_a \). When \( u_*/w_a > 0.35 \), two-dimensional roll structures appear in the velocity fields aligned with the mean wind direction, as shown by the numerical simulation of Sykes and Henn (1989). This change in the turbulent pattern can influence the diffusion process because of the disruption of the horizontal turbulence’s isotropy and the increase of the horizontal velocity variances.

To complete this classification, the stability parameter \(-z_i/L\) is used, following Holtslag and Nieuwstadt (1986), to define the four simulated BL archetypes used in this study: pure CBL (cases B1–B5: \(-z_i/L \geq 40\)), shear–buoyancy-driven BL (cases SB1 and SB2: \( u_*/w_a = 0.25 \) and \( u_*/w_a = 0.35 \), respectively), shear-driven BL (cases S1 and S2: \(-z_i/L \sim 4\) and \( u_*/w_a \sim 0.46\)) and near-neutral BL (case NN: \(-z_i/L \sim 2\) and \( u_*/w_a \sim 0.58\)). The initial conditions and the dimensionless parameters for the simulated cases are summarized in Table 1.
An instantaneous line source (ILS) of scalar (non-buoyant tracer) is emitted along the $x$ axis at two different heights ($z_s/z_i = 0.078$ and $z_s/z_i = 0.48$, where $z_s$ is the release height) after a well-mixed boundary layer has been established (i.e., at the beginning of the fifth hour of simulation). These two emission heights are selected to study the diffusion process from both a “near ground” (i.e., in the surface layer, $z_s < 0.1 z_i$) and an “elevated” release.

The line source measured two grid spacings in the vertical direction and one grid spacing in the horizontal ($y$) direction. The line source can be equivalently interpreted in terms of a continuous point source (CPS) by using the relationship $t = x/u$, as explained by Willis and Deardorff (1981) and Nieuwstadt and de Valk (1987). Because the numerical grid moves with the mean wind along the $x$ direction, this relationship transforms the numerical $x$ coordinate in the physical elapsed time after the release of the scalar. The line source after a certain time $t$ is equivalent to the time evolution of the concentration pattern of a scalar released from a CPS at a certain distance $x = πt$.

For each simulated case, three different realizations are performed in which the horizontal position of the instantaneous release was changed. The results are subsequently ensemble-averaged over the different realizations and the above-mentioned CBL classification.

To analyze the dispersion characteristics of the plumes in the various flows, it is convenient to introduce the statistical parameters used in our study.

The vertical and horizontal dispersion parameters $σ_z$ and $σ_y$ are defined according to Nieuwstadt (1992) as follows:

$$σ_z^2 = \frac{\int (z - \bar{z})^2 c \, dV}{\int c \, dV}$$

and

$$σ_y^2 = \frac{\int (y - \bar{y})^2 c \, dV}{\int c \, dV},$$

where $c$ is the space-dependent concentration, $dV = dx \times dy \times dz$, and $\bar{z}$ and $\bar{y}$ are the mean plume height and the mean plume horizontal position, respectively, defined according to

$$\bar{z} = \frac{\int z \, c \, dV}{\int c \, dV}$$

and

$$\bar{y} = \frac{\int y \, c \, dV}{\int c \, dV}.$$

The spatial integration along the $x$ coordinate is equivalent to the physical time integration, because of the equivalence between ILS and CPS discussed earlier.

Because in many experimental studies [e.g., the water-tank experiments of Willis and Deardorff (1976, 1981)] the vertical dispersion parameter is calculated as the displacement from the source height, rather than from the mean plume height, we computed also this vertical dispersion parameter $σ'_z$, defined as

$$σ'_z^2 = \frac{\int (z - z_s)^2 c \, dV}{\int c \, dV}.$$

The dimensionless crosswind-integrated concentration $C_y$ is calculated (Nieuwstadt and de Valk 1987) by

$$C_y = \frac{z_c}{\int c \, dV} \int c \, dx \, dy.$$

Last, from the concentration’s time series, the concentration fluctuation is derived using

$$σ_i^2 = \frac{\int (c - \bar{c})^2 \, dt}{Δt},$$

where $t = x/u$, $Δt = 1$ h, and time-averaged concentration

$$\bar{c} = \frac{\int c \, dt}{Δt}.$$
3. Dispersion in a pure CBL

In this section, we discuss the dynamics and the dispersion characteristics simulated by means of LES under pure convective conditions (averaged over the cases B1–B5, with $u_\infty < 0.3$). They are presented not only to confirm the correct behavior of the model by comparing them with available laboratory and atmospheric experiments, but also as a reference point for the simulations when shear is introduced.

We first analyze the vertical profiles of the velocity variances because they provide direct information on the flow structure and are directly related to the dispersion parameters. The diffusion characteristics (plume spread and ground concentrations) are next discussed and are compared with the experimental data. Various commonly used parameterizations (interpolations of laboratory or numerical results) designed for buoyancy-driven boundary layers are further compared with the LES results.

a. Velocity variances

Figure 1 shows the profiles of vertical and horizontal velocity variances scaled with the convective velocity scale $w_\infty^2$. The velocity variances are calculated as space (cross horizontal) and time (1 h) averages of the velocity fluctuations. Various experimental data (laboratory and field campaign) are also shown for comparison (Willis and Deardorff 1974; Lenschow et al. 1980; Deardorff and Willis 1985; Caughey and Palmer 1979; as reported by Schmidt and Schumann 1989). The LES results for the SB1–SB2 cases ($u_\infty / w_\infty = 0.3$) are also shown (dashed line).

b. Mean plume height and dispersion parameters

1) Near-ground release

Figure 2 shows the dispersion characteristics (mean plume height and vertical and horizontal dispersion parameters) for a near-ground release ($z_0 / z_i = 0.078$). The dimensionless space (time) is defined as

$$ X = \frac{w_\infty x}{z_i}, \quad t = \frac{w_\infty t}{z_i}. \quad (10) $$

Although the scatter in the “convective dispersion observed with remote sensors” (CONDORS) data (Briggs 1993) is large, the mean plume height calculated by the LES (Fig. 2a) is in satisfactory agreement with the experiments (in particular with the water-tank results).

In Fig. 2b, the LES results for the vertical dispersion parameter, as calculated by both Eqs. (2) and (6), are shown. As mentioned earlier, the two differ in that one uses the release height whereas the other uses the mean plume height in the definition of the vertical dispersion parameter. The LES results are compared with the laboratory data by Willis and Deardorff (1976) and the CONDORS data by Briggs (1993), and they are found to be in good agreement with the experimental data in both cases.

For short times ($X < 1$) the model results fit well with the expression

$$...
as the best fit to many different experimental data (both surface and elevated release). As suggested by Briggs (1985), Eq. (13) might be regarded as the limiting minimum value for the horizontal dispersion parameter for the CBL, with higher values expected in the presence of wind shear. In the same figure, we depict the following relationship derived from experimental data (Grynning et al. 1987):

$$\frac{\sigma_x}{z_i} = \frac{\sigma_0/z_i t}{(1 + t/2T_y)^{3/2}} = \frac{\sigma_0/w_* X}{\left(1 + \frac{X}{2T_y w_*}\right)^{3/2}},$$

which is in excellent agreement with the LES results. The Lagrangian time $T_y$ is parameterized following Nieuwstadt (1992) as

$$T_y = 1.7 \left(\frac{\sigma_x}{w_*} \right)^2 \frac{z_i}{w_*} \sim 300 \text{ s},$$

and is in agreement with the experimental values of Weil et al. (2002).

Although all of the Eqs. (12), (13), and (14) fit the LES results within the standard deviation, we consider that Eq. (14) is the one that includes explicitly the dependence of the dispersion parameters on the turbulence, rather than empirical constants either derived by statistical theory or extrapolated by experimental data.

Last, we discuss the decomposition of the (vertical) dispersion parameters into two components, the meandering ($m_\chi$) and relative ($s_\chi$) dispersions as proposed by Nieuwstadt (1992):

$$\frac{\sigma_\chi}{z_i} = m_\chi^2 + s_\chi^2.$$

The meandering part describes the contribution of the large-scale turbulent eddy motion, and the relative dispersion quantifies the increasing size of the plume caused by small-scale mixing. They are defined as follows:

$$m_\chi^2 = \int (z_i - z)^2 c \, dV$$

and

$$s_\chi^2 = \int (z - z_i)^2 c \, dV,$$

where the local plume height $z_i$ is defined as

$$z_i = \frac{\int z c \, dy \, dz}{\int c \, dy \, dz}.$$

Similar expressions hold for the horizontal components.
which is in good agreement with the parameterization suggested by Lamb (1982) for $X < 2/3$ for elevated releases: $\sigma(z_i) = 0.5X$.

The results for the horizontal dispersion parameter are shown in Fig. 3c. They are very similar to the experimental data obtained by Willis and Deardorff (1981) up to $X = 2$.

Some further considerations can be addressed by comparing the horizontal dispersion results for the near-ground release (Fig. 2c) with the elevated release (Fig. 3c). As pointed out by Briggs (1985) and confirmed by our LES results, the horizontal spread at short distances ($X < 1$) for a near-ground release grows faster than that of the elevated release. This behavior is due to the conversion of vertical motion into horizontal motion at the base of the updrafts and downdrafts near the surface. Despite these differences, Eq. (14) reproduces correctly (within the standard deviation) the horizontal spread for both the releases (near ground and elevated).

On the contrary, at large distances, the LES results have the same values independent of the release height. This result is explained by the fact that the plume released near the ground is rapidly raised up by the updrafts and is above the surface layer at distances $X > 0.3$. Because the vertical profile of $w^2/w_\text{h}^2$ remains constant above the surface layer (see Fig. 1c), one expects similar values of the horizontal parameter for both the near-ground and elevated releases. This situation is consistent with the analysis of Briggs (1993), who shows that the empirical fit of CONDORS data for the near-ground release approaches that for the elevated release as time increases. Lamb (1982) suggested the same empirical formulation for $\sigma(z_i)$ for both near-ground and elevated releases for $X > 1$:

$$\frac{\sigma(z_i)}{z_i} = \frac{1}{3}X^{2/3},$$

which agrees well with our LES results.

c. Nondimensional crosswind-integrated ground concentrations

Figure 4 shows the normalized crosswind-integrated ground concentrations $[C]$, calculated by means of Eq. (7) at $z = 0$ for the near-ground and elevated releases. The cross section of the normalized crosswind-integrated concentrations (contours of $C$, as a function of height) will be shown in the following section (Figs. 8a and 9a). For the near-ground release, the pattern generally agrees with the laboratory results of Willis and Deardorff (1976) and other numerical simulations (Nieuwstadt and de Valk 1987; Lamb 1978). The maximum occurs at $X = 0.25$ in close agreement with the water-tank experiment, and, although the LES results slightly overestimate the data by Willis and Deardorff (1976) and Weil et al. (2002) for $0.25 < X < 1$, they reproduce correctly the slope, which follows the expression:

$$\frac{\sigma(z_i)}{z_i} = 0.52X,$$

which is the following relationship:

$$m_x = \sigma_x t \quad X \ll T_v$$

$$dm_x/dt = 0 \quad X \gg T_v,$$

which implies that $m_x$ approaches a constant value at large distances.

2) Elevated release

In Fig. 3, the dispersion statistics for the plume emitted from an elevated release ($z_i/z_e = 0.48$) are shown. The LES results show a satisfactory agreement with laboratory and experimental data. In Fig. 3b, only $\sigma_x$ [Eq. (2)] is shown because the mean plume height does not differ too much ($\sim 15\%$) from the initial release height (Fig. 3a), and in consequence $\sigma_x$ is similar to $\sigma(z_i)$.

The best fit for the LES results at short times is the following relationship:

$$\sigma(z_i) = 0.52X,$$
surface maximum occurs at $X$, higher values of $X$ to fit our LES results, the curve is shifted toward 1 at large distances. Following Gryning et al. (1987), approaches the uniform vertical mixing asymptote of 0.08 at $X$. This result suggests that the tracer remains near the surface at longer distances from the source, with the minimum occurring at $X = 3.5$ (as can be seen in Fig. 9a in which the cross-wind-integrated concentrations are shown), in agreement with Lamb (1982) and Henn and Sykes (1992). The faster lifting off in the water tank may be explained by a small positive buoyancy acquired by the droplets used in their experiment, as suggested by Willis and Deardorff (1981).

Although we are aware that a complete validation of a numerical model would require a much wider and deeper comparison with experimental data, in this section we showed that the LES results are in good agreement with available experimental data, previous numerical studies, and fitting expressions derived from field campaigns. Therefore, we are confident that the LES is able to simulate dispersion under conditions of pure convection.

4. Dispersion in a buoyancy- and shear-driven boundary layer

We now discuss the results for the CBL driven by both buoyancy and shear. From here on, all of the results are scaled by the velocity scale

$$w_m^3 = w_m^1 + 5u_m^1.$$  (25)

This expression was proposed first by Zeman and Tennekes (1977) on the scaling of the turbulent kinetic energy equation, and it was modified by Moeng and Sullivan (1994) on the basis of their numerical simulation results. The velocity scale $w_m$ takes into account the characteristic velocity scales for both convective- and shear-driven flows as well as providing a suitable scaling for the second-order moments of turbulence (Moeng and Sullivan 1994).

We similarly define the new dimensionless distance (time) as follows:

$$X = \frac{w_m x}{z_i} \frac{t}{z_i},$$  (26)

a. Velocity variances

As in the previous section, we first discuss the LES results for the dynamic variables and then analyze the...
plume dispersion characteristics. The increasing wind shear modifies the turbulent flow structure, and this modification is reflected by the profiles of velocity variances. As pointed out previously, the dispersion parameters are directly proportional to the velocity variances. As a consequence, a correct calculation of these variables is essential to understand and parameterize the behavior of the dispersion characteristics under different flow regimes.

As pointed out by previous studies (Sykes and Henn 1989; Moeng and Sullivan 1994), buoyancy and shear act differently on the turbulence’s structure. The interaction between these two mechanisms results in the disruption of the horizontal isotropy of the flow. According to Moeng and Sullivan (1994), in a CBL driven by both shear and buoyancy the turbulent pattern is peculiarly different from either a pure convective or a neutral situation. In fact, the shear near the ground creates small streaky structures that are lifted up by buoyancy and merged to form two-dimensional rolls in the middle of the CBL.

The effect of shear in the $u$ and $v$ wind components is clearly noticeable in Fig. 5, in which the profiles of the velocity (fluctuation) variances are shown for the run classified according to increasing wind shear (see section 2). Numerical simulations (Sykes and Henn 1989; Moeng and Sullivan 1994) and wind-tunnel measurements (Fedorovich et al. 2001, not shown) show similar profiles of $\langle u^2 \rangle$ and $\langle v^2 \rangle$ characterized by the presence of maxima at the bottom and top of the CBL. In these regions, in fact, the energy is transferred from the vertical scale to the horizontal scale, because the thermals are influenced by the shear and the presence of the boundaries. As shown in Fig. 5a, another important feature is the reduction of the vertical velocity variance by the increasing of wind.

**Fig. 5.** Dimensionless vertical profiles of the velocity variances calculated by the LES are shown for all cases: B1–B5 (continuous line); SB1–SB2 (dashed line); S1–S2 (dotted–dashed line); and NN (dashed–dotted–dotted–dotted line). For comparison, the numerical results of Moeng and Sullivan (1994) for their SB1 case ($u^*/w^*_m \sim 0.6$) are also shown ( ).

**Fig. 6.** (a) Mean plume height, (b) vertical dispersion parameter, and (c) horizontal dispersion parameter for a near-ground release for all of the cases as calculated by the LES as function of the dimensionless distance (time) $X_m$ defined by Eq. (26). In (b) the neutral limit [Eq. (27)] (long-dashed line) is shown.

b. Mean plume height and dispersion parameters

1) NEAR-GROUND RELEASE

Figure 6 shows the statistics of the dispersion process (mean plume height and vertical and horizontal dispersion parameters) for the near-ground source for all of the simulated CBLs, averaged according to the classification discussed above. As pointed out by Mason (1992) and Gopalakrishnan and Avissar (2000), the mean effect of the increasing wind speed is reduction of the vertical mixing. This reduction is related to the decrease in the value of the vertical velocity variance profiles, discussed previously.

The mean plume height and the vertical spread (Figs. 6a,b) show similar characteristics. As the wind speed increases, the tracer is lifted up more slowly because it is advected horizontally by the wind. As explained previously, the presence of the ground reduces the vertical motion so that the vertical spread grows slowly for the near-ground releases. For the NN case ($-z_i/L = 1.8$) the buoyancy is too weak to lift up the tracer and, in consequence, it remains close to the surface. The vertical spread grows almost linearly up to a distance of $X_m = 1$, and only at very large distances does it slowly reach an asymptotic limit as the tracer is spread all over the layer. For short distances ($X_m < 1$), the growth of $\sigma_z^2/z_i$ is consistent with the neutral limit proposed by Briggs (1985),

$$\frac{\sigma_z^2}{z_i} = 0.64 \frac{u^*_w t}{z_i} = 0.64 \frac{u^*_w}{w^*_m} X_m \sim 0.28 X_m .$$  \hspace{1cm} (27)
which is also shown in the figure. The growth of $\sigma_i/z_i$ for the intermediate cases (SB and S1–S2) lies between the two extreme situations, pure buoyancy and near neutral, in agreement with other numerical results by Mason (1992) and Gopalakrishnan and Avissar (2000). A parameterization that encompasses all of the cases, from pure buoyancy to a neutral situation, will be presented and discussed in the next section.

In Fig. 6c the results for the horizontal spread ($\sigma_y/z_i$) are shown. As the wind shear increases, the horizontal spread is enhanced and, in the near-neutral cases, its value can double that for the pure convective cases, in agreement with the research conducted by Mason (1992) and Luhar (2002).

To determine the importance of the shear contribution, we can study the effect of wind shear on the horizontal dispersion by decomposing (Venkatram 1988)

$$\sigma_y^2 = \sigma_{s_b}^2 + \sigma_{s_y}^2,$$  \hfill (28)

where $\sigma_{s_b}$ refers to the buoyancy-generated dispersion and $\sigma_{s_y}$ is the contribution due to the change in the wind direction with height (shear-generated dispersion). A parameterization for the shear contribution was proposed by Luhar (2002) for coastal fumigation models. In the next section, we will use that approach to develop a parameterization for the horizontal dispersion in a buoyancy- and shear-driven boundary layer, and it will be compared with the LES results.

2) Elevated release

Figure 7a shows the mean plume height for all of the simulated cases for an elevated release. The B1–B5 and SB1–SB2 cases show a very similar pattern, whereas in the S1–S2 cases the minimum in the mean plume height is reached at farther distances away from the sources ($X_m = 1.7$), because the tracer is advected horizontally by the wind and simultaneously transported downward. Moreover, in the near-neutral case, the mean plume height does not show a sensible displacement from its initial value, because the tracer is scarcely influenced by the thermal forcing.

The vertical and horizontal dispersion parameters are shown in Figs. 7b and 7c, respectively. They have the same general behaviors as previously discussed for the near-ground release for all of the cases. The vertical spread for short times ($X_m < 0.5$) is generally consistent with the Taylor’s law

$$\frac{\sigma_y}{z_i} \approx 0.51 \frac{w_m}{w_i} X_m,$$  \hfill (29)

as shown for the near-neutral case.

The horizontal spread is enhanced, and, far enough away from the source ($X_m > 1$), its value is similar to that for the near-ground release, as discussed previously for the pure convective cases.

c. Crosswind-integrated and ground concentrations

1) Near-ground release

Figures 8a–d show the crosswind-integrated concentrations $C_y$ for the near-ground release. The relative ground concentrations are shown in Fig. 8e. Concentration $C_y$ is strongly affected by the relative importance of buoyancy and shear. In fact, as the shear-buoyancy ratio increases, the tracer is advected horizontally for a longer time before being lifted up by the thermals. In the SB case, the pattern is somewhat similar to the pure convective BL; an elevated maximum is present at $X_m = 2$ but the surface minimum is now extended to $X_m = 3.5$. In the S1 and S2 cases (Fig. 8c), the tracer is transported by the wind for a long time before being lifted up by the weak buoyancy. A surface minimum is present at $X_m = 3$, but the relative elevated maximum is not evident. In the NN case, the wind is so dominant that it keeps the tracer close to the ground even at a large distance from the source.

This behavior has an important effect on the ground concentrations, as shown by Fig. 8e. All of the simulated cases show a similar concentration maximum at $X_m = 0.25$. In fact, at very short distances ($X_m < 0.2$) the plume is still in the surface layer, as shown by Fig. 6a. In this region, the vertical structure of turbulence is similar in all of the cases, as shown by the value of the vertical velocity variance close to the surface (Fig. 5a). The vertical dispersion parameter (Fig. 6b) also shows similar value in all the stability regimes for $X_m < 2$.

At greater distances from the source ($X_m > 0.2$), the different contribution of thermal and mechanical turbulence strongly modifies the vertical dispersion (as
shown in Fig. 6b) and, as a consequence, the ground concentration, which increases markedly with the wind speed. A common asymptotic value is reached around $X_m = 4$ when the tracer is uniformly spread within the mixed layer.

2) ELEVATED RELEASE

Figure 9 shows the crosswind-integrated and ground concentrations for the elevated release. As for the near-ground release, the increasing wind and the simultaneous reduction of the buoyancy affect the plume dispersion, which shows different behaviors according to the increasing shear–buoyancy ratio.

The SB1 and SB2 cases show the same general pattern as the pure buoyancy condition, but the elevated minimum that was visible for the pure convective cases ($X_m = 1$, $z/z_i = 0.75$; Fig. 9a) is now no longer present (Fig. 9b), and the maximum ground concentration is shifted to a greater distance from the source ($X_m \sim 1.3$; see Fig. 9e). The buoyant force starts raising the plume at $X_m = 2.5$, and a ground minimum is visible around $X_m = 3.4$. In the S1 and S2 cases, the ground maximum is shifted farther toward large distances ($X_m = 1.8$) and no surface minimum is found, proving that the buoyancy is unable to raise the tracer after it has reached the ground. In the near-neutral regime, the plume shows a typical Gaussian behavior, the tracer remains elevated even at large distances, and no surface maxima are present.

4) Meandering and relative dispersion in buoyancy- and shear-driven boundary layers

As shown previously, the vertical dispersion parameter can be represented as the sum of the meandering and relative diffusion components, according to Eq. (16). The results in a pure CBL have already been discussed by Nieuwstadt (1992), but the investigation of the relative importance of meandering and relative dispersion in the case of weak convection is still missing.

In Fig. 10, the ratio between the meandering component and the relative diffusion ($m_z/s_z$) is shown as a function of the distance $X_m$ from the source for all of the simulated cases. As shown by Nieuwstadt (1992), the meandering is important, especially at short distances at which the plume motion is governed by the thermals. After reaching a maximum, the meandering component rapidly decreases, because the plume motion...
The ratio of meandering to relative dispersion \( \frac{m}{s} \) calculated by the LES for all of the simulated cases for the (a) near-ground and (b) elevated releases.

For a near-ground release (Fig. 10a), we note that the contribution of the meandering to the vertical spread is always less important than the relative diffusion. The meandering is reduced by the increasing wind shear, especially at short distances \( X_m < 1 \). This result is explained by the presence of the ground, which limits the vertical motion; as the wind increases and the buoyancy diminishes, the tracer remains close to the surface for a longer time before being lifted up, and so the vertical motion (meandering) remains limited.

For the elevated release (Fig. 10b), the plume motion in the pure convective flow is dominated by the meandering at short distances \( m/z_i > 1 \), in agreement with the results of Nieuwstadt (1992). As the wind increases, it reduces the vertical motion, but for \( X_m < 0.75 \) the meandering still remains the principal contribution to the vertical spread; in fact, as discussed previously, the wind profile shows a strong shear only near the ground, which means that in the middle of the BL the buoyancy force is still the main driving process in the plume dispersion.

e. Concentration fluctuations

The study of the concentration fluctuations has a great importance in the atmospheric dispersion problems because they can be of the same order of magnitude as the mean concentrations. The valuation of the concentration uncertainty was investigated in the past either in convective conditions or in neutral flows by laboratory experiments (Fackrell and Robins 1982; Deardorff and Willis 1984; Weil et al. 2002) and numerical simulations (Henn and Sykes 1992; Sykes and Henn 1992). From the concentration fields calculated by the LES, the value of the concentration fluctuation intensities is explicitly calculated [Eq. (8)] and is compared with the experimental results. It is unfortunate that, because the fluctuation intensity depends strongly on the source size (Fackrell and Robins 1982) and, moreover, the results in the literature for the neutral scale were scaled with different length and velocity scales, only a qualitative comparison is carried out.

The relative concentration fluctuation intensities \( \sigma_c/\overline{C} \) on the plume centerline at ground level are shown in Fig. 11a and 11b for the near-ground and elevated releases, respectively.

For the elevated release (Fig. 11b), the results for the near-ground release (Fig. 11ab) in the B1–B5 cases show that the concentration fluctuation intensity decreases with the distance from the source, similar to results for the experimental data. However, they underestimate the water-tank data by Deardorff and Willis (1984) and Weil et al. (2002) because of the differences in the values of the source size and release height \( z_s/z_i = 0.134, z_s/z_i = 0.15, \) and \( z_s/z_i = 0.078 \) for Deardorff and Willis (1984), Weil et al. (2002), and our study, respectively. The source size and the ratio between it and the eddy size, in particular, are the main factors that determine the value of the maximum, as explained by Henn and Sykes (1992). Our initial plume size (instantaneous line source) is determined by the vertical
grid length (varying from 25 to 50 m), and it may be larger than the eddy size at this source height, resulting somehow in an underestimation of the fluctuation maximum.

The major source of concentration fluctuation is the meandering of the plume, as explained by Fackrell and Robins (1982). As the wind shear increases, the meandering and, as a consequence, the concentration fluctuations are reduced. In the NN situation, a nearly constant value is found at each distance from the source, consistent with the wind-tunnel data by Fackrell and Robins (1982) (around 0.5).

The results for the elevated release (Fig. 11b) are in a very good agreement with the numerical experiment by Henn and Sykes (1992), and a marked maximum is found at $X_{m} = 0.3$. This result is consistent with the maximum in the meandering component shown in Fig. 10b. In fact, for the elevated release, the vertical motion of the plume is dominated at short distances by the large eddies. Similar to the previous discussion, the reduction of the plume is dominated at short distances by the large eddies. Similar to the previous discussion, the reduction of the plume is dominated at short distances by the large eddies.

### 5. Parameterization for the dispersion in buoyancy- and shear-driven boundary layers

In this section, parameterizations for the dispersion parameters $\sigma_x$ and $\sigma_y$ are proposed. These expressions are evaluated for all of the simulated flows. Although many studies are available in either the pure convective or neutral limit, attempts to parameterize the behavior of the plume in buoyancy- and shear-driven BLs are scarcer (Briggs 1985). The dispersion parameters are directly related to the velocity variances whose vertical profiles change with the increasing wind shear because of the change in the turbulent structure (Fig. 5).

Below, we propose parameterizations that include the combined effect of buoyancy and shear on dispersion. The parameterizations can be used to calculate the plume dispersion in conditions of relatively flat terrain and homogeneous land surfaces.

#### a. Horizontal dispersion parameter

As stated previously, the veering of wind direction with height increases the horizontal dispersion, according to Eq. (28) in which the shear contribution ($\sigma_{v}$) is added to the buoyancy-generated dispersion ($\sigma_{b}$) calculated by Eq. (14). Different expressions have been proposed for the shear-generated horizontal spread, which are written below in a general form as

\[
\sigma_{x}^2 = aS_{z}\tilde{f}(\sigma_{y}^2T_{w}^{'^s}T_{w}^{'^b}),
\]

where $t$ is time, $T_{w}^{'}$ is the Lagrangian time for the vertical turbulent velocity, and $a$ is a constant. The coefficients $b$, $c$, and $d$ determine the curve’s slope, ranging from a cubic tendency at small values of $t$ ($b = 2$, $c = 3$, and $d = 1$) to a linear tendency at large times ($b = -2$, $c = 1$, and $d = -1$). In our study, the nondimensional wind direction shear $S_{w}$ is defined, following Luhar (2002), as

\[
S_{w} = \frac{V}{w_{m}}\theta_{m},
\]

where $\theta_{m}$ is the difference between the geostrophic wind direction and the wind direction at the mean plume height, and $V$ is the total wind intensity ($V^2 = u'^2 + v'^2$) at the same height.

Explicit testing of the expressions represented in Eq. (30) is rare by either field campaign or numerical models, and therefore our LES results could be useful in deriving and evaluating a suitable parameterization for horizontal dispersion under shear conditions.

As discussed previously, the buoyancy-generated dispersion can be satisfactorily parameterized with Eq. (14), whereas the shear contribution is calculated by rearranging the formula proposed by Luhar (2002) as follows:

\[
\sigma_{x}^2 = \frac{a_{0}S_{z}^{2}a_{w}^{2}T_{w}X_{m}z_{i}/w_{m}}{\left[1 + \left(\frac{X_{m}}{X_{0}}\right)^{2/3}\right]^{2/3}}.
\]

Equation (32) is an interpolation between the cubic ($X_{m}$) and linear ($X_{0}$) dependences on $X_{m}$ that were discussed previously. The distance $X_{0}$ marks the transition between the two tendencies, from cubic to linear, and is defined as

\[
X_{0} = \left(\frac{z_{i}^{2}}{a_{b}a_{0}^{2}w_{m}^{2}T_{w}/\tau_{s}}\right)^{1/2}w_{m}/z_{i}.
\]

From the LES results, $X_{0}$ ranges from 2.7 in the SB1–SB2 cases to 3.3 in the near-neutral situation. The value of the constants $a_{0}$ and $b_{0}$ are fixed to 0.09 and 60, respectively, and $\tau_{s} = 0.7z_{i}/w_{m}$, following Luhar (2002).

Figure 12a shows the value of $\sigma_{x}$ calculated by Eq. (28) compared with the LES results. We found a good agreement for all of the cases studied. Figure 12b shows the shear contribution only, compared with the total dispersion for the pure buoyancy cases (in this case, $\sigma_{x} = \sigma_{b}$ because the shear is absent). Our results show that for large values of the wind, the shear contribution is of the same order of magnitude or is larger than the buoyancy-generated dispersion, in agreement with the analysis of Luhar (2002).

#### b. Vertical dispersion parameter

The vertical spread is strongly dependent on the source height (Weil 1988). For an elevated release, the dispersion parameter at short times must follow Taylor’s law:

\[
\frac{\sigma_{z}}{z_{i}} = \frac{\sigma_{x}}{w_{*}}X_{i}.
\]
For a near-ground release, on the contrary, the presence of the ground converts the vertical motion into horizontal motion. Therefore, the vertical spread is reduced, and the growth departs from linearity. Moreover, as discussed previously, the increasing of the shear–buoyancy ratio produces a wind profile characterized by strong shear near the BL boundaries (surface and entrainment zone), whereas in the middle of the layer the \( u \) component of the wind remains constant with height.

For this reason, we propose two different parameterizations for \( \sigma_z \), depending on the release height. The vertical dispersion parameter for a source above the surface layer (elevated release) can be successfully represented by the formula

\[
\frac{\sigma_z}{z_i} = \frac{\sigma_z}{w_b} X = 0.51 \frac{w_b}{w_m} X_m, \tag{35}
\]

which fits our LES results accurately.

For a near-ground release, at short distance from the source (\( X_m < 0.5 \)), two opposite effects have to be taken into account: the reduction of the vertical spread because of the surface and the increasing contribution produced by the shear. Notice that, to facilitate the use of the parameterization, the vertical dispersion parameter is calculated as the displacement from the source height [Eq. (6)] rather than from the mean plume height. As shown previously [Eq. (11)], in the pure CBL (\( u_b \sim 0 \)) the growth of \( \sigma_z/z_i \) follows

\[
\frac{\sigma_z}{z_i} = 0.52 X^{6/5} \tag{36}
\]
in the pure convective limit, whereas in the near-neutral case the vertical spread grows linearly according to

\[
\frac{\sigma_z}{z_i} = 0.6 \frac{u_b}{w_m} X_m. \tag{37}
\]

The constant 0.6 is the best fit for our results, and it is consistent with the field campaign neutral limit \( \sigma_z = 0.64 u_b t \) that was indicated by Briggs (1985).

In the intermediate cases, in which buoyancy and shear are acting simultaneously, the LES results show that the vertical spread growth falls in between the two limits (Fig. 6b). In consequence, we suggest a parameterization that combines Eqs. (36) and (37):

\[
\frac{\sigma_z}{z_i} = \left[ \left( 0.52 \frac{w_b}{w_m} \right)^{12/5} X_m^{2/5} + \left( 0.6 \frac{u_b}{w_m} \right)^{2/3} \right]^2, \tag{38}
\]

where the function \( f \) depends on the atmospheric surface layer stability, according to

\[
f = \left[ -0.2 \frac{z_i}{L} \right]^{-3} \left[ 1 + \left( -0.2 \frac{z_i}{L} \right)^{-3} \right]. \tag{39}
\]

Equation (38) has the correct limits for the pure buoyancy (\( -z_i/L \to \infty \) and \( f = 1 \)) and neutral limits (\( -z_i/L = 0 \) and \( f = 0 \)) discussed above. The weighting function \( f \) [Eq. (39)] accounts for the reduction of vertical spread with shear already noticed in previous work (Mason 1992; Gopalakrishnan and Avisser 2000). However, to our knowledge, this is the first time a parameterization that explicitly accounts for this effect is presented and evaluated.

In Fig. 13, the parameterization [Eq. (38)] is compared with the LES results for all the simulated cases at short distances (\( X_m < 1 \)). According to Briggs (1985), parameterizations for the vertical dispersion parameter are valid only when \( X_m < 0.7 \) because at greater distances, when the tracer is lifted off by the thermals, the vertical distribution becomes non-Gaussian. At greater distances (\( X_m > 2 \)), when the tracer is uniformly mixed, the vertical spread reaches a constant value (about 0.55), as shown in Fig. 6. As shown in Fig. 13, Eq. (38) reproduces correctly the LES results at short distances (\( X_m < 0.6 \)) for all of the cases.

6. Conclusions

The dispersion of a passive scalar in boundary layers driven by different combinations of buoyancy and shear was investigated by means of a large-eddy simulation and was evaluated with laboratory and field observations. Four boundary layer archetypes varying from pure convection to a near-neutral situation were simulated and was evaluated. To our knowledge, this is the first time a parameterization that explicitly accounts for this effect is presented and evaluated.

In Fig. 13, the parameterization [Eq. (38)] is compared with the LES results for all the simulated cases at short distances (\( X_m < 1 \)). According to Briggs (1985), parameterizations for the vertical dispersion parameter are valid only when \( X_m < 0.7 \) because at greater distances, when the tracer is lifted off by the thermals, the vertical distribution becomes non-Gaussian. At greater distances (\( X_m > 2 \)), when the tracer is uniformly mixed, the vertical spread reaches a constant value (about 0.55), as shown in Fig. 6. As shown in Fig. 13, Eq. (38) reproduces correctly the LES results at short distances (\( X_m < 0.6 \)) for all of the cases.
focused on the values of the dispersion parameters, ground concentrations, and concentration fluctuations.

A good agreement between the LES results and the laboratory and field experiments was found in the pure convective situation.

The influence of the increasing wind shear was first studied on the flow statistics (profiles of velocity variances) because the dispersion characteristics are directly dependent on the turbulence’s properties. The results show an increase in the horizontal velocity variance and a reduction in the vertical velocity variance.

The main effect of the wind shear on dispersion statistics results in a reduction of the vertical spread, whereas the horizontal spread is enhanced. As a consequence, the ground concentrations are strongly influenced and the LES results show that the increasing wind tends to advect the plume horizontally for a longer time. The tracer therefore reaches the ground at greater distances from the source. For the near-ground releases, at very short distances the ground concentrations show a similar behavior in all of the simulated flows. This result is explained by the fact that for $X_m < 0.3$ the tracer is still in the surface layer where the turbulent and dispersion statistics ($\sigma_u / w_m$ and $\sigma_z / z_i$) have similar values for all the stability regimes. At greater distances ($0.3 < X_m < 3$), the plume is strongly affected by the different ratio between the thermal and mechanical forcing, and the ground concentrations increase markedly with the increasing wind shear. At $X_m > 3$ the tracer is uniformly spread within the mixed layer and a common asymptotic value for the ground concentration is found.

The meandering component of the vertical dispersion is also modified by the wind shear, in particular, near the ground where the presence of the surface tends to enhance the shear, which reduces the looping of the plume. This reduction is especially visible at short distances from the source ($X_m < 1$) where the plume motion is influenced by the large turbulent eddies and the meandering is the main contribution to the vertical dispersion.

Because meandering is the main source of concentration variance, the maximum of the concentration fluctuations is shown to diminish as the flow becomes less convective. Although the differences in source size and release height do not allow a direct comparison, the LES results agree qualitatively with the experimental results in both convective and neutral conditions.

Parameterizations for the dispersion parameters that account for the combined effect of buoyancy and shear were proposed. The parameterization for $\sigma_y$ is partially based on a previous study by Luhar (2002) in which the wind rotation was explicitly considered in the shear-generated dispersion. The parameterization of $\sigma_z$ accounts for two opposite effects: the reduction of the vertical motion near the ground and the shear-generated turbulence. Both of the parameterizations give satisfactory results when compared with the LES data in all of the simulated cases, and they will be further tested in operational models for dispersion.

Acknowledgments. The authors thank Stefano Galmarini for many useful discussions and comments. Author A. Dosio is funded within the Centre of Expertise Emissions and Assessment—a cooperation between TNO and Wageningen University.

APPENDIX

List of Symbols

- $C_y$: Crosswind-integrated concentration
- $c$: Concentration of the passive tracer
- $\bar{c}$: Time-averaged concentration
- $g$: Acceleration of gravity
- $L$: Monin–Obukhov length
- $m_x$: Meandering component of the dispersion in the horizontal direction
- $m_z$: Meandering component of the dispersion in the vertical direction
- $S_\theta$: Dimensionless shear
- $s_y$: Relative dispersion in the vertical direction
- $T_x$: Lagrangian time for the horizontal turbulent velocity
- $T_w$: Lagrangian time for the vertical turbulent velocity
- $u$, $v$, $w$: Wind components
- $\langle u^2 \rangle = \sigma_u^2$: Horizontal ($u$) velocity variance
- $u_f$: Friction velocity
- $U_g$: Geostrophic wind
- $V$: Total mean wind
- $\langle v^2 \rangle = \sigma_v^2$: Horizontal ($v$) velocity variance
- $\langle w^2 \rangle = \sigma_w^2$: Vertical velocity variance
Cuijpers, J. W. M., and P. G. Duynkerke, 1993: Large eddy simulation