Dispersion of a Gaseous Plume in the Sheared Convective Boundary Layer: Evaluation of a Lagrangian Particle Model Versus Wind Tunnel Simulation Data

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INTRODUCTION

The anisotropic and skewed turbulent motions on a broad scale range contribute to the complexity of dispersion patterns in the atmospheric convective boundary layer (CBL). The main turbulence forcing in the CBL is the convective heat transfer from a warm underlying surface. Several field, numerical and laboratory studies, see *e.g*. Eberhard *et al*. [1], Willis and Deardorff [2], [3], [4], Weil *et al*. [5], Nieuwstadt [6] and Mason [7], have shown that this buoyant forcing generates vertical up- and downward motions that lead to the characteristic looping behavior of gaseous plumes in the CBL. In the presence of mean wind, shear contribution to the turbulence production becomes important, especially in the near-surface portion of the CBL. There are very few experimental data available on the dispersion parameters in the sheared CBL, and most of existing CBL dispersion models have been evaluated using data from water tank simulations of the shear-free CBL.

Extensive data sets of mean flow, turbulence and dispersion characteristics in a horizontally evolving CBL have been obtained by Fedorovich *et al*. [8] and Fedorovich and Thäter [9] in a thermally stratified wind tunnel of the University of Karlsruhe (UniKa), Germany. They found that wind shears can essentially modify the CBL turbulence dynamics. In the present study, concentration patterns from the UniKa wind tunnel simulations of gaseous tracer dispersion in the sheared CBL are compared with results from a 3-D Lagrangian stochastic particle dispersion model (LPDM) described in Rotach *et al*. [10] and de Haan and Rotach [11]. This dispersion model satisfies the well-mixed condition continuously in the range from stable to convective conditions and accommodates pollution sources located at arbitrary heights within the boundary layer. To account for interacting mechanisms of shear and buoyant turbulence production, the probability density function (pdf) of the particle velocities in the model is constructed as a weighted sum of a neutral pdf (horizontal and vertical velocity fluctuations are correlated and jointly Gaussian) and a convective pdf (skewed vertical velocity fluctuations non-correlated with the horizontal velocity fluctuations).

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METHODS OF INVESTIGATION

As basic case for the comparison with LPDM simulations, data sets from the point-source tracer experiments in the wind-tunnel CBL flow over a relatively smooth underlying surface and in the absence of elevated wind have been selected. Two different source heights, a ground-level release and a source at $z = 0.1\text{m}$, which is about 30% of the inversion elevation, have been considered (see also Thaeter *et al*. [12]). The LPDM runs have been performed for atmospheric CBL flow that is a scaled analog of the one simulated in the wind tunnel. The basic parameters describing the wind-tunnel flow and its atmospheric counterpart are summarized in Table 1. As similarity criteria the Richardson number $Ri_{\Delta T}$ based on the temperature difference across the inversion layer and the ratio between shear stress and convective velocity have been used. The length scale ratio is given by $LSR = z_{i,Atm.} / z_{i,WT} = 2000$.

Table 1. Scaling parameters of the wind-tunnel CBL flow and its atmospheric counterpart.

	Wind tunnel	Atmosphere
Mean mixed layer wind velocity u in m/s	1.00	11.55
Shear stress velocity u_* in m/s	0.076	0.88
Convective velocity w_* in m/s	0.18	2.08
Mixed layer height z_i in m	0.35	700.00
Monin-Obukhov length L in m	-0.067	-133.6
Roughness length z_0 in m	0.0001	0.20
Temperature difference across the inversion layer ΔT in K	30.00	2.00

Besides the spatial distributions of pollutant concentration, the wind tunnel experiments have provided high resolution data on the CBL mean flow parameters and turbulence statistics. Additional information on the flow characteristics has been available from numerical simulations of the horizontally evolving CBL with a LES code presented in Fedorovich *et al*. [13]. The wind tunnel and LES mean flow and turbulence profiles have been compared with the parameterized profiles employed in the LPDM.

The mean wind profile measured in the wind tunnel has been well represented by the LPDM mean wind profile. However, significant differences have been observed between the measured and parameterized (according to [10]) turbulence statistics. A comparison of the normalized velocity variances is presented in Fig. 1. Since measurements have not been available for the lateral velocity component *v*, LES data from the study by Fedorovich *et al*. [13] (gray lines) have been employed. For each velocity component, two profiles measured approximately 2.3 m and 4 m downwind of the tracer source location have been considered, which are very close to each other. Accordingly, this part of the CBL flow may be considered as approximately horizontally homogenous. For the longitudinal (*u*) and vertical (*w*) velocity component variances, the LES results agree well with the measured data (symbols). The LES results for the variances of the lateral velocity component *v* have been very similar to the variances of the *u* component. For these two velocity components, the LPDM parameterizations (black dashed lines) provide significantly larger values over the main portion of the CBL. In the case of the *w* component, differences between the LPDM profile and wind-tunnel data have been mainly observed in the upper part of the CBL close to the inversion layer. Comparisons of the turbulent momentum flux and third moment of the vertical velocity component are presented in Fig. 2. It is obvious that the LPDM parameterization of the turbulent shear stress describes the wind tunnel data fairly well, whereas the peak of the third moment of *w* has been significantly underestimated by the LPDM parameterization.

Thus, two LPDM runs have been conducted and analyzed for each source configuration: (*i*) run A with the original turbulence parameterizations of the LPDM given in Tab. 2 by Eqs. (1a)-(4a), and (*ii*) run B with modified profiles represented by Eqs. (1b)-(4b) in Tab. (2) that have been fitted against the wind tunnel data. The modified profiles are shown by the black solid lines in Figs. 1 and 2. The influence of the differences between measured and parameterized profiles on the dispersion characteristics will be discussed in the next section.

Table 2. Comparison of turbulence parameterizations employed in the LPDM (left column) and profiles fitted against the turbulence data measured in the wind tunnel (right column). Only turbulence characteristics that have been modified for the present study are listed.

Original LPDM parameterization (Run A)		Modified profile (Run B)	
$\frac{\overline{u'^2}}{w_*^2} = 0.35 + \frac{u_*^2}{w_*^2}\left(5 - 4\frac{z}{z_i}\right)$	(1a)	$\frac{\overline{u'^2}}{w_*^2} = 0.1 + \exp\left\{-3\sqrt{\frac{z}{z_i}}\right\}$	(1b)
$\frac{\overline{v'^2}}{w_*^2} = 0.35 + \frac{u_*^2}{w_*^2}\left(2 - \frac{z}{z_i}\right)$	(2a)	$\frac{\overline{v'^2}}{w_*^2} = 0.1 + \exp\left\{-3\sqrt{\frac{z}{z_i}}\right\}$	(2b)
$\frac{\overline{w'^2}}{w_*^2} = 1.5\left(\frac{z}{z_i}\right)^{2/3} \exp\left\{-2\frac{z}{z_i}\right\} + \frac{u_*^2}{w_*^2}\left(1.7 - \frac{z}{z_i}\right)$	(3a)	$\frac{\overline{w'^2}}{w_*^2} = \left(0.27 + 14\left(\frac{z}{z_i}\right)^{1.6}\right) \cdot \exp\left\{-4.4\frac{z}{z_i}\right\}$	(3b)
$\frac{\overline{w'^3}}{w_*^3} = 1.3\left(\frac{z}{z_i}\right)\left(1 - \frac{z}{z_i}\right)^2$	(4a)	$\frac{\overline{w'^3}}{w_*^3} = 2\left(\frac{z}{z_i}\right)\left(1 - \frac{z}{z_i}\right)^{1.2}$	(4b)

DISPERSION PATTERNS

Comparisons of vertical concentration profiles downwind of the ground-level and elevated point source normalized by Deardorff scales are shown in Figs. 3 and 4. The LPDM results and measured concentration values agree fairly well. However, for both source locations the results of the LPDM runs underestimate the measured concentration levels in the near field of the source, meanwhile further downwind over-predictions by LPDM are observed. The modification of the turbulence parameterizations employed in LPDM for run B result only in a slightly better agreement of measured and calculated concentration profiles. In the case of the ground-level source the rising of the plume, which has been observed in the wind tunnel, is not reproduced by both LPDM runs. In the upper part of the CBL, close to the inversion layer, LPDM predicts to large concentrations if the condition of total reflection at $z = z_i$, which has been originally used, is applied. For run A realistic values are obtained if only 50% of the particles are reflected meanwhile for run B the best agreement with the wind tunnel data is found without reflection of particles at the inversion layer. These results indicate that entrainment at the inversion layer is an important process that needs to be further studied and appropriately represented in the dispersion model. The differences observed close to the sources might be triggered by discrepancies of the source design in the wind tunnel and its representation in LPDM. Furthermore it must be taken into account that in this region the wind tunnel CBL flow still horizontally develops, meanwhile horizontal flow homogeneity has been assumed in the LPDM calculations.

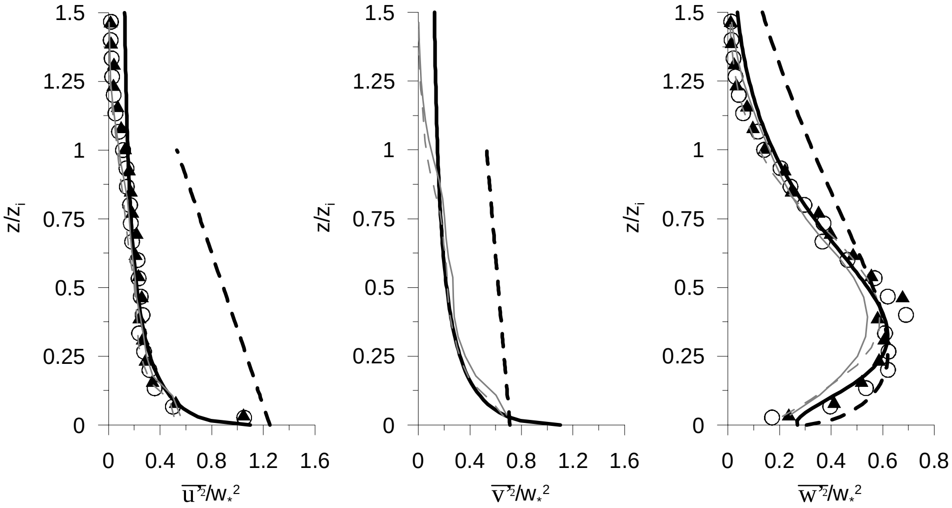

Figure 1. Measured (symbols) and parameterized (dashed black line) variances of the longitudinal (left plot), lateral (central plot) and vertical (right plot) velocity components. The modified LPDM profiles are shown as black, solid lines. The gray lines correspond to results of LES of the wind-tunnel CBL performed by Fedorovich *et al.* [13].

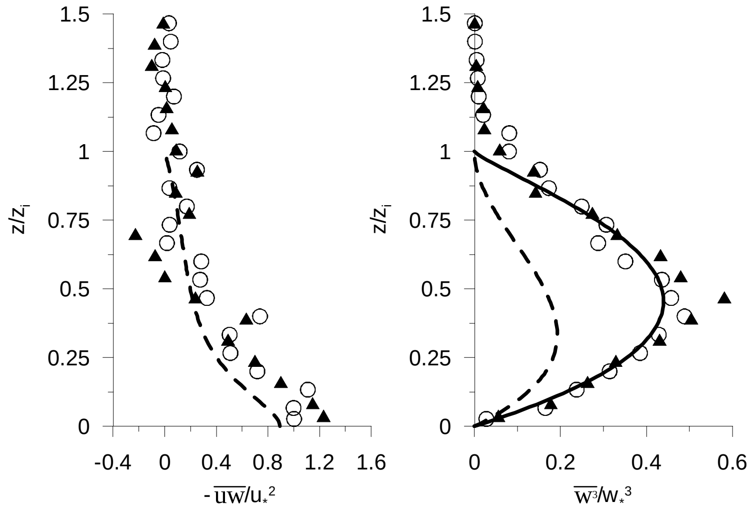

Figure 2. Measured (symbols) and parameterized (dashed black line) momentum flux (left plot) and third moment of the vertical velocity component (right plot). The modified LPDM profiles are shown as black, solid lines.

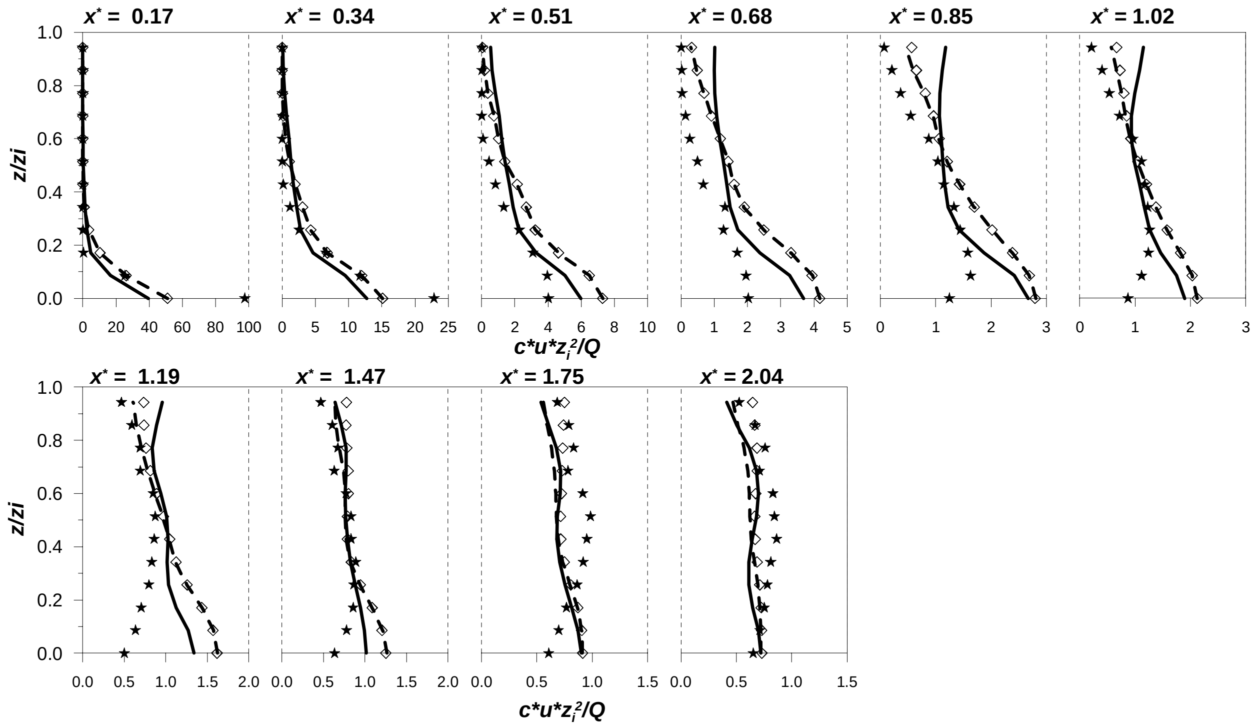

Figure 3. Comparison of measured (stars) concentration profiles downwind of a ground-level point source with LPDM calculations. Dashed lines correspond to run A results with 50% of the particles reflected at the inversion layer and solid lines to run B results without particle reflection at the inversion layer. Results for Run A with total reflection at the inversion layer are shown by the diamonds. All quantities are normalized by Deardorff scales.

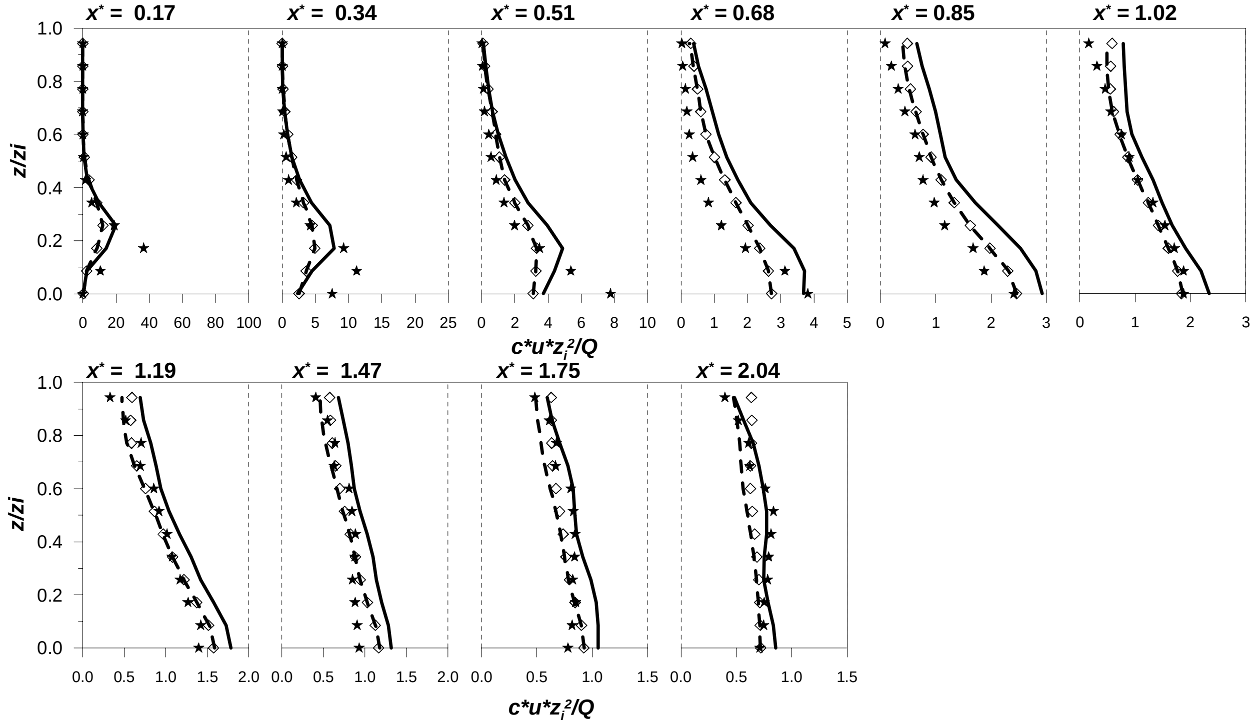

Figure 4. Same as Figure 3 but for an elevated point source.

SUMMARY

The Langrangian stochastic particle model LPDM did a fairly good job in predicting concentrations patterns in CBL flow influenced by wind shears. Entrainment at the inversion layer has been proved to be an important parameter and its incorporation in the dispersion model needs to be further investigated. The model predictions could be slightly improved by modifications of the LPDM turbulence parameterizations that better represent the measured turbulence characteristics. The influence of the horizontal flow development on the dispersion process and its integration in the dispersion model will be further studied and comparisons for situations with increased roughness elements are planned.

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