LARGE EDDY SIMULATION OF AIR POLLUTION DISPERSION IN A HIGHLY CONVECTIVE BOUNDARY LAYER

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Abstract. *This work describes the time evolution of three-dimensional structure of an inert and passive atmospheric pollutant emitted by instantaneous line source in a highly Convective Boundary Layer (CBL). The CBL properties were numerically simulated using a large eddy simulation model developed by Moeng(1984) and modified by Sullivan et al. (1994). Under quasi-steady equilibrium conditions, the statistic properties of simulated turbulent flow are in agreement with others observational and numerical studies using LES. Despite the low horizontal velocity conditions the resulting plume follows the typical spatial pattern observed in convection tank experiments and other numerical simulations for elevated source height.*

Keywords: *LES model, highly convective boundary layer, pollutant dispersion.*

1 – INTRODUCTION

The dispersion models represent an important tool in the investigation of pollutants transports in the planetary boundary layer (PBL) as long as they are validated against data. Unfortunately, information of atmospheric dispersion in the PBL with appropriate resolution and accuracy is very difficult to obtain. This is especially difficult in third world countries, like Brazil, where the air pollution impact assessments are carried out by operational diffusion models not validated for local conditions.

An alternative approach to fill this observational gap that will be explored in this work, is the LES model. This type of model allows a very precise description of turbulent eddies that transport most of pollutants in the PBL (Deardorff, 1972; Nieuwstadt and Valk, 1987; Rizza et al., 2003). Even though they require considerable computational effort, LES model has become more popular in air pollution research applications even for complex topography and heterogeneous land-use conditions (Gopalakrishnan and Avissar, 2000; Walton et al., 2002).

The results simulated here are compared with the results of Willis and Deardorff (1976a, 1978). It is quite common to use the convection tank experiment result to validate the LES simulations, where the plume generated near to the surface by a continuously emitting point source, propagates upward in a CBL. Inversely, a release away from the surface propagates downward.

In this work the plume vertical dispersion is investigated for a horizontally homogeneous highly CBL under low horizontal wind velocity (U) conditions. This condition is quite restrictive and precludes the application of the Taylor's hypothesis to transform the release time (t) in downstream distance (X_*) (Willis e Deardorff, 1976b; Nieuwstadt and Valk, 1987).

2 – METHODOLOGY

Two simulations were carried out using the LES model version developed by Moeng (1984) and modified by Sullivan et al. (1994). The total time of the simulations was of the order of 1500 time steps (corresponding to about 1.2 hours of CBL time evolution), with 80 by 80 by 80 grid points, covering a numeric domain of 5 km by 5 km by 2 km in x, y and z, respectively. The initial and boundary conditions correspond to intense thermal convection associated to a surface sensible heat flux of 230 W m^{-2} and very small wind shear condition. When these conditions are used, the LES model is able to generate highly CBL over a range of stability of $-z_i/L = 585$ and $-z_i/L = 800$, where z_i is the PBL height and L is the Monin-Obukhov length scale. These stability conditions correspond to the observed ones in São Paulo City during most of the year (Oliveira et al., 2003).

The results presented hereafter are based on the three-dimensional fields generated by LES after the first 1000 time steps, when the CBL has reached a state of quasi-equilibrium steady. At this time (t_0) all pollutant is released along of a line parallel to x-axis (instantaneous line source), located at y = 2.5 km and in two different vertical levels, $z_s = 0.20\,z_i$ and $z_s = 0.45\,z_i$. The crosswind integration of pollutant concentration for instantaneous line source and continuous point source are equivalent (Willis and Deardorff, 1976b; Nieuwstadt and Valk, 1987). The spatial distribution of the concentration of pollutant at t_0 is gaussian in order to minimize spurious and negative concentration values inherent to the numerical approach used in this version of the LES (Cai, 2000). The gaussian distribution is also a fair representation of the concentration field of a pollutant released instantaneously over a line source at its initial stage of evolution in the atmosphere.

3 – RESULTS AND DISCUSSION

The turbulent flow in the CBL is characterized by asymmetric structures composed of updraft and downdraft. The updrafts are originated in the surface and remain confined to narrow regions as they move towards the top of the CBL. The downdrafts spread over broader regions of the CBL gradually descending downward to the surface (Lenschow and Stephens, 1980). These structures can be identified in the instantaneous fields of the vertical wind velocity (w') and potential temperature (θ') fluctuations around the horizontal average values. For instance an updraft flow, corresponding to the dark area between $2500\,\text{m} < x < 3000\text{m}$, occupies the entire vertical extension of CBL (Fig. 1a). Near to the top of the CBL the updraft loses its initial buoyancy, but it has enough turbulent kinetic energy (TKE) to penetrate in the inversion layer, pushing down the air (downdraft) with larger potential temperature from the stable layer above to the CBL. The entrainment warmer air generates positive fluctuations of θ' near to the top, $750\text{m} < z < 1250\text{m}$, indicated by dark areas in Fig. (1b).

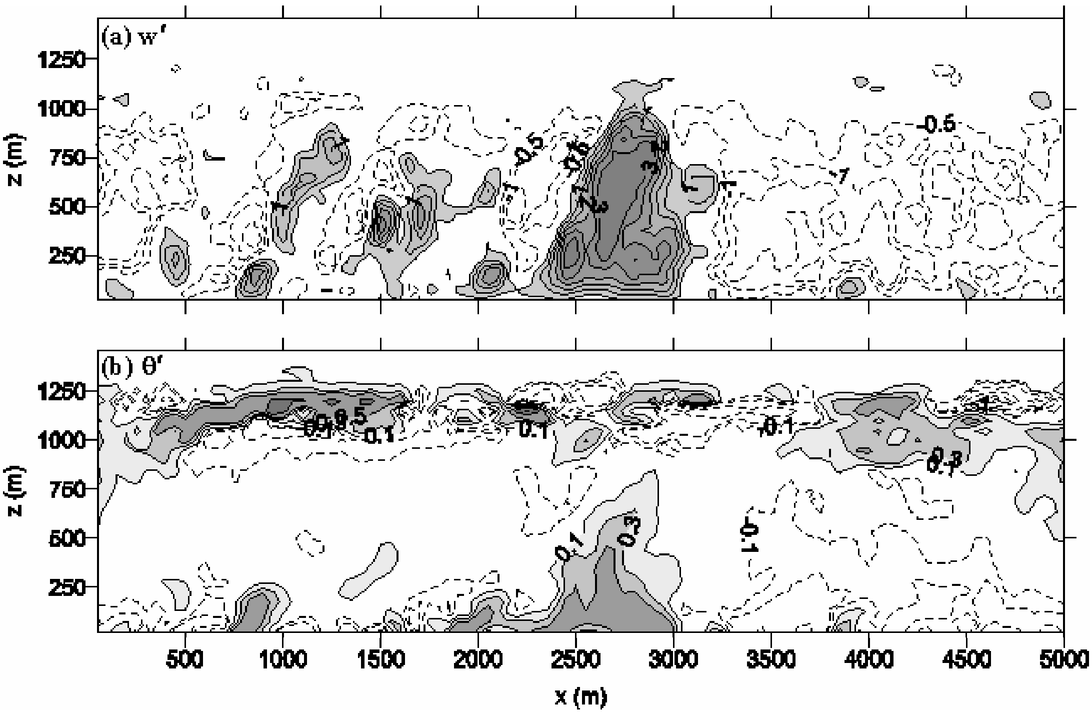

Figure 1 - Contour in the vertical plane: (a) vertical velocity and (b) potential temperature.

The degree of asymmetry in the CBL turbulent flow is indicated by the skewness parameter. In the case of vertical velocity (Fig. 2), $\left(\langle w'^3\rangle / \langle w'^2\rangle^{3/2}\right)$ is positive in most of the CBL vertical extent indicating that the vertical wind field is characterized by large areas of weak downdrafts and small areas of strong updrafts. The negative spurious values near to the surface are caused by the inability of subgrid model to represent the turbulent process near the surface in this version of the LES model (Schmidt and Schumann, 1989; Moeng and Rotunno, 1990). To minimize the effects of negative skewness the first grid point level of the model was not taken into consideration in the estimates of concentration field displayed in this work.

The results obtained for instantaneous line source can be alternatively interpreted in terms of continuous point source plume diffusion. Such interpretation is based on the application of the Taylor´s hypothesis $\left(t_T = x/U\right)$, where the release time $\left(t\right)$ can be associated at the longitudinal distance x. However, the horizontal velocity of the simulations ($U \leq 1$ m s^{-1}) is out the validity limit suggested by Willis and Deardorff (1976b) for application of the Taylor´s hypothesis.

Therefore, it was necessary to use the release time $\left(t\right)$ in substitution the Taylor´s time scale $\left(t_T\right)$. In this way, the downstream distance $\left(X_*\right)$ is given for: $X_* \approx \frac{w_*}{z_i} t$ instead of $X_* \approx \frac{w_*}{z_i}\frac{x}{\overline{U}}$, where w_* is the velocity scale of the CBL.

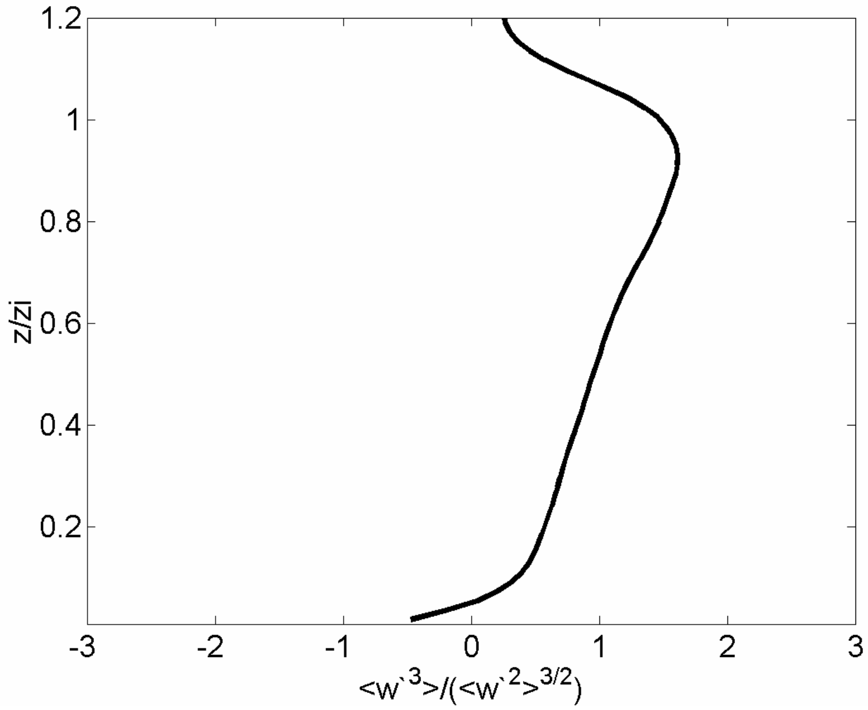

Figure 2 - Vertical profile of the vertical velocity skewness.

Figures (3a) and (3b) show dimensionless crosswind-integrated concentration obtained from source located at $z_s = 0.20\,z_i$ and $z_s = 0.45\,z_i$, respectively. The maximum concentration $\left(c_{max}\right)$ descends and reaches the surface as consequence of the downdraft effects. This maximum remains in the surface during a small distance, moving upwards progressively as effect of the updraft. In the Fig. (3a), c_{max} stays in the surface for a distance $\Delta X_* \approx 0{,}4 \quad \left(0{,}4 \leq X_* \leq 0{,}8\right)$ equivalent to the plume obtained for Willis and Deardorff (1978).

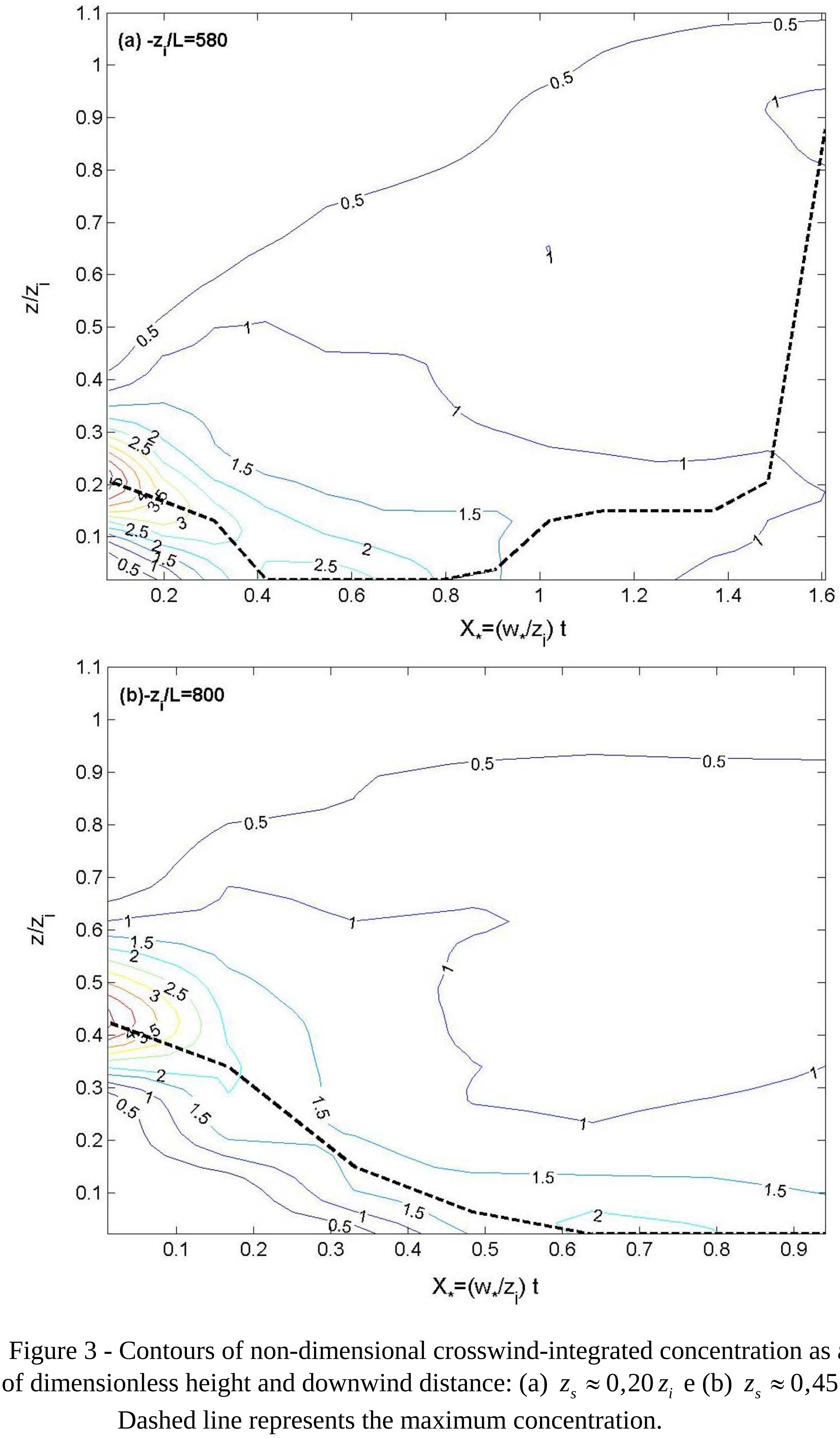

Figure 3 - Contours of non-dimensional crosswind-integrated concentration as a function of dimensionless height and downwind distance: (a) $z_s \approx 0{,}20\, z_i$ e (b) $z_s \approx 0{,}45\ z_i$. Dashed line represents the maximum concentration.

For the source located in middle of the CBL (Fig. 3b) the concentration is maximum in the surface at $X_* \approx 0{,}6$, in agreement with the results presented by Henn and Sykes (1992). However due to the small simulation time, in this case is not possible to estimate the distance that c_{max} stays near to the surface.

According to Lamb (1984), the phenomenon that causes the plume descending movement near to the elevated sources is the asymmetry of the probability density function (pdf) of the vertical velocity in the horizontal plane. In Fig. (4) the pdf of the non-dimensional vertical velocity is presented in the respective emission source levels. The results are in agreement with the non-gaussian pattern of the pollutant vertical dispersion in the CBL (Willis and Deardorff, 1976a, 1978; Lamb, 1984; Weil, 1988). In spite of the larger area of the horizontal plan to be dominated by downdrafts $(\approx 60\%)$, the skewness of the vertical velocity is positive, once that the updrafts are more intense (as observed in Fig. 2).

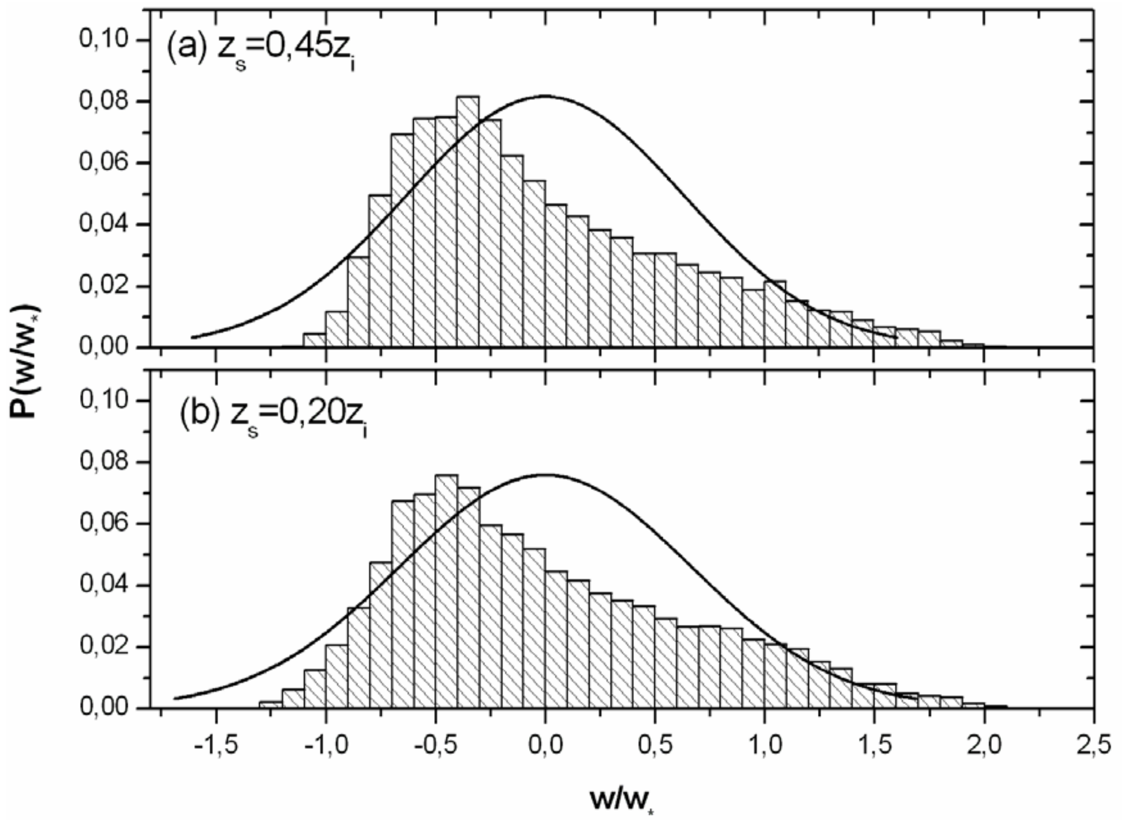

Figure 4 - Probability density of vertical velocity: (a) $z_s \approx 0{,}45\,z_i$ e (b) $z_s \approx 0{,}20\,z_i$.
Solid line represented the gaussian pdf.

4 – CONCLUSIONS

In this work the LES model was used to study the dispersion of pollutant released from elevated source heights. The plume was generated using an instantaneous line source located in two different vertical levels, $z_s = 0.20\,z_i$ and $z_s = 0.45\,z_i$. Despite the low horizontal velocity condition of the simulations ($U \leq 1$ m s^{-1}) the used methodology was capable to reproduce the typical spatial pattern observed in convection tank experiments and others numerical simulations.

For elevated source heights, the maximum concentration occurs in the surface before propagating for the higher layers. This pattern reflects the asymmetry in the vertical velocity pdf in the horizontal plane, indicating the largest probability of downdraft occurrences $(\approx 60\%)$.

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