LARGE EDDY SIMULATION OF CARBON MONOXIDE IN THE CITY OF SÃO PAULO

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INTRODUCTION

The city of São Paulo, with about 11 millions habitants, together with 39 other smaller cities, forms the Metropolitan Region of São Paulo (MRSP). This region is occupied by 20.5 millions of habitants and has approximately 7 millions of vehicles. São Paulo is located about 60 km far from the Atlantic Ocean. The MRSP has an area of 8051 km^2 and it is the largest urban area in South America and one of the 10 largest in the world (Codato *et al.*, 2007).

These areas are characterized by highly populated cities that are emitting considerable amounts of pollutants, in special carbon monoxide (CO). For instance, the MRSP has emitted about 1,460,000 ton of carbon monoxide (CETESB, 2005). Approximately 98% of this emission is due to 7 million vehicles, and under low wind conditions a considerable fraction of this CO remains in the metropolitan area generating highly concentrations in intense traffic regions.

Air pollution is the most important environmental problem in São Paulo. There are indications that long term exposure to high levels of pollutants has caused dramatic public health problems. There are also evidences that pollution in São Paulo has even altered the local climate by affecting the diurnal evolution of diffuse, direct and global solar irradiance components at the surface (Codato *et al.*, 2007).

Objective

The objective of this work is to investigate the statistical properties of the convective planetary boundary layer (PBL) over a homogeneous urban surface using the large eddy simulation (LES) model developed by Moeng (1984). Here, special attention will be given to the characterization of turbulent transport of pollutant at the top of the PBL during daytime.

Observations have indicated that the diurnal evolution of CO in São Paulo has a progressive decreasing o the CO concentration at the surface level (Fig. 1a). Considering the idealized diurnal evolution of CO flux (Fig. 1b), based on vehicles traffic inventory, one may conclude that the decreasing in the CO concentration after 10 LT (Local time) may be related to the entrainment of clean air in the top of the PBL.

Therefore, it will be investigated in this work how the entrainment of clean air in the top of the PBL during the period of time PBL reaches maximum vertical evolution - around noontime - affects the observed decreasing in the CO concentration at the surface.

NUMERIC MODEL

The numerical simulation of turbulent flows is carried out in LES solving directly the large eddies (resolved-scale). The small-scale part of the turbulent flow (subgrid-scale) is solved indirectly by using parameterization techniques. This version LES model was developed by Moeng (1984).

The LES code has been used by the Group of Micrometeorology in the University of São Paulo to simulate the PBL properties for highly convective conditions (Marques Filho, 2004). It was also used to investigate the pollution dispersion by considering a continuously emitting area and point sources located at the surface (Marques Filho, 2004; Marques Filho *et al.*, 2007).

The numerical simulations in this work were carried out using a parallel version of LES code. It was run in a cluster HP-Compaq S45, from the Laboratory of Computation of the University of São Paulo (LCCA-USP).

Initial and boundary conditions
The domain used in the numerical simulation was formed by 128 by 128 by 128 grid points in x, y and z, respectively, covering 10 km by 10 km by 2 km.

The model was run for 25 thousand time steps. The numerical stability is verified every computational time step in agreement with the Courant-Friedrichs-Lewy condition. In the simulations carried out here the time step was around 0.5 seconds, corresponding to a total time of about 4 hours of PBL time evolution. It required about 100 hours of CPU time in the cluster HP-Compaq S45.

The initial conditions for pollutant concentration and potential temperature correspond to a mixed layer with vertical extension of 1000 m. The initial mixed layer potential temperature was 300 K and pollutant concentration was 5 ppm. Above 1000 m, potential temperature increases 9 K in the inversion layer (around 100 m) and increases about 3 K km^{-1} in the free atmosphere above. The vertical variation of CO concentration in the inversion layer is consistent with CO concentration equal to zero ppm in the free atmosphere. The vertical profiles of horizontal velocity components (u, v) are assumed to be constant and equal to a zonal geostrophic wind of 5 m s^{-1}.

The surface sensible heat flux was set 240 W m^{-2} (Marques *et al*, 2004), and the pollutant surface flux was set equal to zero ppm m s^{-1}. They were kept constant throughout the simulation. These conditions were defined in order simulate the time evolution of PBL during noontime (between 10 and 14 Local Time) in a realistic but simple way. Aerodynamic roughness parameter is set equal to 0.16 m, corresponding to the urban value of roughness (Marques *et al.*, 2007).

Quasi-steady equilibrium
The turbulent flow in PBL reaches a quasi-steady equilibrium when its properties vary with a time scale smaller than the time scale of the boundary conditions and external forcing variations. Under this condition, the PBL statistical properties can be determined as a function of the PBL characteristic scales, which in turn are defined as a function of the boundary conditions, external forcing and the intrinsic turbulent flow characteristics (Sorbjan, 1986).

The time evolution of the normalized TKE averaged over the entire PBL $\langle\langle E\rangle\rangle / w_*^2$ as a function of the dimensionless time t/t_* (Fig. 2). After $t/t_* \approx 4$ (vertical dash), $\langle\langle E\rangle\rangle / w_*^2$

becomes approximately constant and equal to 8.2, indicating that the PBL turbulence simulated by LES reaches the quasi-steady equilibrium at about the same time.

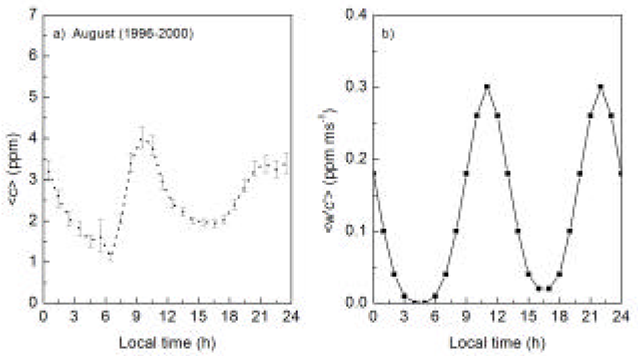

Fig. 1; Diurnal evolution of a) monthly-average values of carbon monoxide in the São Paulo during August, b) idealized vertical flux of carbon monoxide. Hourly values observed during 1996 to 2000.

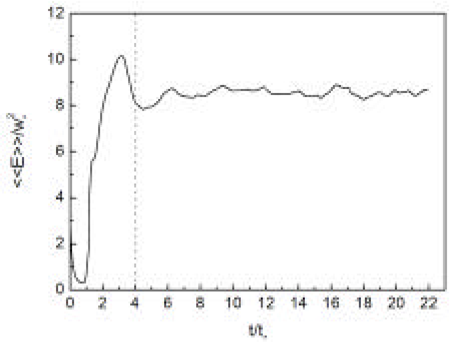

Fig. 2; Time evolution of normalized TKE integrated in the PBL. The characteristic scales are indicated in Table 1.

RESULTS AND CONCLUSION

The results presented hereafter are based on the three-dimensional fields generated after the first 25000 time steps (approximately 4 hours). The statistics were obtained using the model output after PBL has reached a state of quasi-equilibrium (Fig. 2).

The vertical profiles of potential temperature (Fig. 3a), zonal component of wind (Fig. 4a), CO concentration (Fig. 6a) are ensemble average obtained of six and seven outputs, separated by 1,000 time steps each. Important to emphasize that time step was around 0.5 seconds. Similar procedure were carried out for vertical turbulent fluxes of sensible heat (Fig. 3b), horizontal wind components (Fig. 4b) and CO concentration (Fig. 6b), and for the variances of wind components (Fig. 5a-b).

The Obukhov length (L), PBL height (z_i), stability parameter ($-z_i/L$) and the characteristic scales of velocity (w_*), time (t_*) and potential temperature (T_*), simulated numerically by LES every 1 hour are indicated in Table 1.

Table 1. PBL characteristic scales. Numerical simulation results.

Time of simulation	L (m)	z_i (m)	$-z_i/L$	w_* (ms^{-1})	t_* (s)	T_* (K)
1 hour	-25.3	1079	43.2	2.03	532.2	0.12
2 hour	-22.0	1092	49.8	2.03	532.2	0.12
3 hour	-19.1	1121	58.9	2.05	532.2	0.12
4 hour	-17.5	1153	65.7	2.07	562.2	0.12

It is interesting to observe that during the four hours of simulation the stability parameter was within interval $40 = - z_i /L = 70$. Therefore the simulations correspond to typical convective conditions.

Figure 3 indicates the vertical profiles o potential temperature and the respective vertical flux of sensible heat. There one can see all major features of a typical convective PBL, i.e. mixed layer with close to zero vertical gradients of potential temperature and a linearly decreasing profile of sensible heat flux.

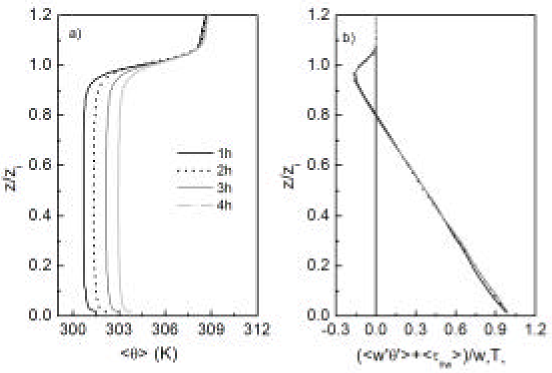

Fig. 3; Vertical profiles of potential temperature and sensible heat flux at 1h, 2h, 3h and 4 hours of simulation.

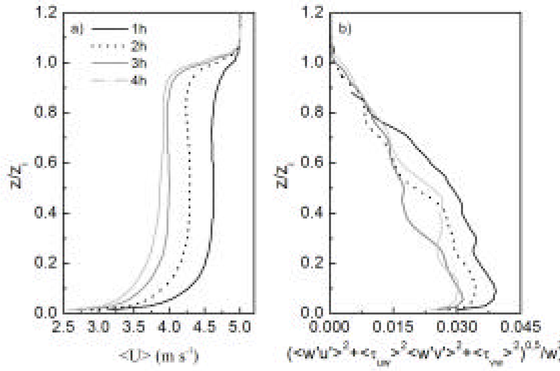

Fig. 4; Vertical profiles of wind speed and vertical flux of momentum at 1h, 2h, 3h and 4 hours of simulation.

Equivalent behavior was obtained for the vertical profiles of zonal component of wind, which decreases with time and show small values of vertical gradient in most of the PBL (Fig. 4a). The vertical flux of horizontal momentum components does also vary linearly with height (Fig. 4b) as expected for barotropic PBL.

Vertical profiles of variance of horizontal and vertical component of wind (Fig. 5a) behaved as expected for convective conditions. The two maxima, located respectively at the surface and near to the PBL top, are consistent with the strong vertical shear present in these two regions of the PBL (Fig. 4a). The maximum in the vertical profile of variance of the vertical wind are located around z/z_i around 0.39 is also consistent results obtained in other simulations (Marques, 2004; Deardorff, 1974).

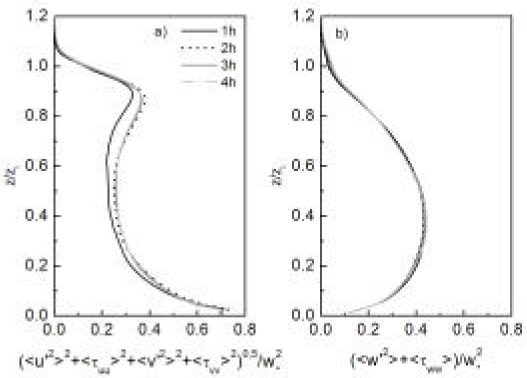

Fig. 5; Vertical profiles of wind speed and vertical flux of momentum at 1h, 2h, 3h and 4 hours of simulation.

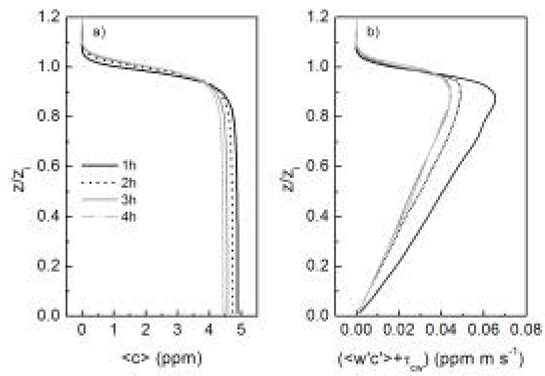

Fig. 6; Vertical profiles of wind speed and vertical flux of momentum at 1h, 2h, 3h and 4 hours of simulation.

The time evolution of the CO concentration simulated numerically indicate a progressive and persistent decreasing due exclusively to the entrainment of clean air at the top of the PBL (Fig. 6a). The vertical distribution of turbulent CO fluxes are reflects this cleaning process undertaken by the PBL, with flux divergence in the entire PBL (Fig. 6b).

Figure 7a indicates that the time evolution of modeled CO concentration follows the observed (monthly average during August) in São Paulo. The comparison between the CO fluxes at the top of the PBL and at the surface, this later estimated based on CETESB inventory (CETESB, 2005), show the importance of the entrainment in the diurnal evolution of the CO concentration in the City of São Paulo. Therefore, to simulate numerically the CO evolution it is important to incorporate the entrainment mechanism in the top of the PBL. Next step will be to run the model using the estimated surface CO flux indicated in Fig. 1b.

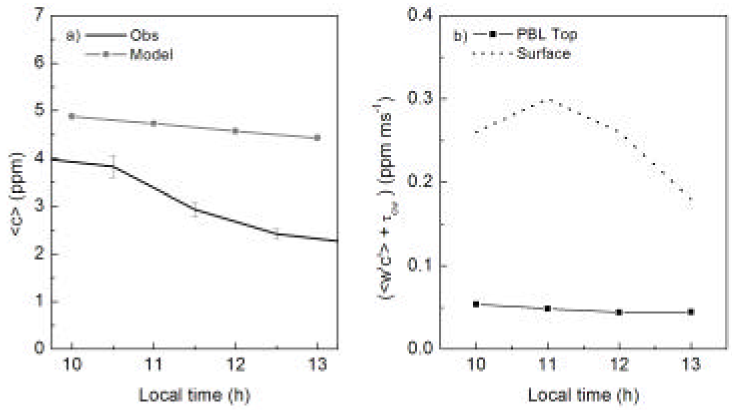

Fig. 7; Time evolution of simulated and observed (a) CO concentration at the surface and (b) CO-flux simulated at the top of the PBL and estimated at the surface from CETESB inventory.

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