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Simulating the characteristic patterns of the dispersion during sunset PBL

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ABSTRACT

A diffusion equation limit derived from the Langevin stochastic particle model is used to study the dispersion of scalars caused by an evolving turbulence in the transition process occurring during the sunset period. Therefore, the random displacement equation is employed to simulate the cross-wind concentrations of pollutants released from low and high point sources. Turbulence inputs are parameterized to describe in a continuous manner the dispersion effects produced by a decaying convective elevated and a shear-dominated stable surface turbulence. The simulation results show that for the initial stage of the sunset transition phenomenon, the pollutants are transported rapidly to the surface. On the other hand, for the sunset evolution advanced stages, the dispersion process happens in a deep stable boundary layer (SBL), in which the pollutants can travel long distances practically without reaching the surface. The major progress shown in this analysis is the description of the transport properties associated to decaying convective eddies in the residual layer (RL). The study shows that the diffusion effects associated to these decaying convective eddies strongly influence the dispersion of scalars during the sunset transition period.

1. Introduction

The turbulence in the planetary boundary layer (PBL) is a complex physical phenomenon, which is in a process of continuous evolution controlled by the action of different forcings (Sorbjan, 2007). An important example of this evolving turbulence is associated to the transition process that happens daily in the layer at sunset. About 1 h before sunset over land, the surface heat flux progressively decreases and, then, during night time becomes negative and, consequently, a stable boundary layer (SBL) develops near the ground (Goulart et al., 2003; Pino et al., 2006). Above this SBL in the Residual Layer (RL), the convective energy-containing eddies start to lose their strength and mixing capacity and the convective boundary layer (CBL) begins to decay. Turbulence decay in the CBL has been investigated by Goulart et al. (2003) using the dynamical equation for the energy density spectrum and by Nieuwstadt and Brost (1986), Sorbjan (1997), Beare et al. (2006), Pino et al. (2006) and Sorbjan (2007) employing LES models. Furthermore, Caughey and Kaimal (1977), Grant (1997), Acevedo and Fitzjarrald (2001), Grimsdell and Angevine (2002), Lapworth (2003) and Anfossi et al. (2004) reported some experimental results about of this sunset transition time.

The dispersion of pollutants by turbulent flows is of central importance in a number of environmental problems. Thusly, the investigation and the use of diffusion mathematical models for the analysis of environmental impact conditions have revealed to be of fundamental value in the assessment of air quality in a large range of distinct scales. In the recent years, a great deal of work has been done to study the airborne pollutant dispersion in convective and stable PBLs. However, the dispersion of pollutants occurring around the evening transition was put aside and most of the diffusion models focused on the CBL under idealized quasi-

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Table 1
Simulation time (t) and SBL height according expression ($h = 70\sqrt{t}$).

t (s)	900	1800	2700	3600	4500
h (m)	35	50	60	70	80

steady conditions, characterized by a constant surface heat flux. Indeed, less attention has been paid to the dispersion in the residual layer, where the diffusion of pollutants occurs in conditions of decaying convective turbulence. It was mentioned that Desiato et al. (1998), simulating the ETEX I long range tracer dispersion experiments with two Lagrangian particle models, obtained the best results when the dispersion in the RL was also included.

The decay of energy-containing eddies in the CBL is the physical mechanism that can sustain, in a robust way, the dispersion process in the RL. To our knowledge, there are no conclusive turbulence observations and studies concerning the dispersion process associated to the release of pollutants happening around the evening transition, where near the surface layer there is the development of the SBL, and above this, the convective eddies that start to decay in the RL. It is important to note that around the evening transition, all the high stacks release pollutants at heights comparable to or interacting with the layer of transition between SBL and RL. This sunset transition time regularly happens on a daily basis and for this situation the investigation of the turbulence diffusion process in this particular period can be employed to evaluate the impact of air pollutants on urban and agricultural environment.

From the above-mentioned discussed arguments and motivated by the scarceness of experimental studies as well as the lack of detailed data about the observed pollutant concentration during the night-day evolution process, it is investigated the turbulent transport process occurring around the evening transition. Therefore, the focus of this study is to simulate the characteristic patterns of the turbulent dispersion of pollutants released from a continuous point source in a diffusive PBL characterized by a decaying convective elevated and stable surface continuous turbulence. To accomplish this analysis, the starting point is the random displacement equation (solution for the asymptotic Langevin equation), in which the turbulent effects are represented by eddy diffusivities for a SBL (Degrazia et al., 2000) and for a decaying turbulence in the CBL (Goulart et al., 2007). The use of these convective decaying eddy diffusivities in air quality models will generate realistic turbulent patterns associated to the sunset transition time. Generally, in this transition state, operational dispersion models consider only the stable turbulent parameterization.

Incorporating the diffusive action associated to the decaying turbulence, happening in the PBL around the evening transition, it is feasible to adequately estimate the air pollution for this particular time period. Throughout this transition period, dispersion models shall incorporate turbulent parameters that present distinct diffusive properties acting simultaneously to dilute the pollutants concentration. Thusly, with these parameterizations (stable below and convective decaying turbulence aloft), the random displacement equation can be used to evaluate, in a quantitative manner, the influence of the decaying convective eddies on the concentration field of pollutants released by high continuous point sources during the sunset transition time and the first hours of SBL development. Finally, it is important to note that in the present study we are dealing with inert pollutant without any chemical reaction or plume rise involved, and as a consequence the changes in concentration are only due to dispersion processes.

2. Turbulence parameterization in the sunset transition time

In the PBL turbulent dispersion models, the selection of an adequate parameterization plays a fundamental role to evaluate the pollutants concentration in the atmosphere. Therefore, the efficiency of each approach, to reproduce correctly the pollutants concentration field, depends on the manner in which turbulent parameters are related to dynamical and thermodynamic evolving properties of the PBL. As a consequence, eddy diffusivities which are used in the random displacement equation are properties of the turbulent environment and are described in terms of the physical quantities that characterize the magnitude of the dispersion in a PBL. Hence, the aim of this section is to show and discuss the eddy diffusivities that have been employed in the random displacement equation to simulate the concentration field of pollutants by a high continuous point source during the sunset transition time. For this reason, it is necessary to parameterize the turbulent transport in a shear-dominated stable PBL (occurring near the ground) and the decaying convective elevated turbulent dispersion (associated to the residual layer).

2.1. Parameterization of the shear-dominated stable turbulence

Turbulent dispersion in a shear-dominated stable PBL is generated close to the ground by mechanical processes that are related to wind shear. In a stable PBL there is a competition between wind shear generated turbulence and stabilizing effects of stratification. Therefore, in our description of the dispersion of pollutants in the sunset transition time, a stable surface layer is considered, in which a continuous turbulence and a negative turbulent heat flux coexist (Nieuwstadt, 1984).

The following relationships for longitudinal, lateral, and vertical eddy diffusivities K_i ($i = u,v,w$) derived by Degrazia et al. (2000), represent the turbulent diffusion in a shear-dominated stable PBL:

$$K_i = C_i \frac{(1-z/h)^{3/4} u_*}{1 + 3.7\left(\frac{z}{L(z-z/h)^{5/4}}\right)} \quad (1)$$

in which $C_x = 4.94, C_y = 1.04$ and $C_z = 0.41$, L is the Obukhov length, u_* is the surface layer friction velocity and h is the height of the stable layer. The magnitudes of the C_i coefficients in the numerator of Eq. (1) show that the eddy vertical motion is strongly limited by the positive stratification.