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Comparison between Eulerian and Lagrangian semi-analytical models to simulate the pollutant dispersion in the PBL

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Abstract

In this work we display a numerical comparison, under statistical and computational point of view, between semi-analytical Eulerian and Lagrangian dispersion models to simulate the ground-level concentration values of a passive pollutant released from a low height source. The Eulerian approach is based on the solution of the advection–diffusion equation by the Laplace transform technique. The Lagrangian approach is based on solution of the Langevin equation through the Picard's Iterative Method. Turbulence inputs are calculated according to a parameterization capable of generating continuous values in all stability conditions and in all heights of the Planetary Boundary Layer (PBL). Numerical simulations and comparisons show a good agreement between predicted and observed concentrations values. The comparison reveals the main advantages and disadvantages between the models.

Keywords: Model comparison; Lagrangian model; Eulerian model; Laplace transform technique; Picard's Iterative Method; Model evaluation

1. Introduction

Lately, the pollutant dispersion in the Planetary Boundary Layer (PBL) has been simulated by an Eulerian approach, solving in a semi-analytical fashion, the diffusion–advection equation by the Laplace transform technique. The main idea consists of the following steps: stepwise approximation of the eddy diffusivity in the z variable, the Laplace transform application in the set of resulting advection–diffusion equation with constant eddy diffusivity, solution of this set using standard results, determination of integration constants by the application of boundary and interface conditions and, finally, the reconstruction of the pollutant concentration by a

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numerical Laplace transform inversion approach namely the Gaussian–Legendre quadrature scheme. A wide class of problems of pollutant dispersion simulation in the PBL has been solved by this methodology, among then we mention the works of Vilhena et al. [1], Moreira et al. [2], Degrazia et al. [3] and Mangia et al. [4].

On the other hand, recently was proposed a Lagrangian model that simulates the pollutant dispersion in the PBL solving, also in semi-analytical manner, the Langevin equation by the Method of Successive Approximations or Picard's Iterative Method. The Picard Method is an iterative numerical process that can approximate the solution of an initial problem value. The method generates a sequence of functions that converges to a unique solution of the initial problem value. Picard's Iterative Method can be used to solve any differential equation and it has been considered in many applications in physics, mathematics and engineering. The Lagrangian model is obtained considering the Gram–Charlier Probability Density Function (PDF) of turbulent velocity, through which Gaussian and non-Gaussian turbulence conditions can be considered. This model has been evaluated through the comparison with experimental data and results obtained by other dispersion models [5].

In this work, motivated by the semi-analytical character of the mentioned approaches, in the sense that no approximation is made in the derivatives appearing in the diffusion equation and Langevin equation, we focus our attention to the following question: which model, Eulerian or Lagrangian, is the best one to simulate the pollutant dispersion in the PBL? To answer this question, we report a numerical comparison, under statistical and computational point of view, between the Eulerian and Lagrangian results for the pollutant concentration. The turbulent parameters used as input in Eulerian model (eddy diffusivities) and Lagrangian model (wind velocity variances and Lagrangian decorrelation time scales) are parameterized according to a scheme able to generate continuous values in all stability and in all heights in the PBL. Ground-level concentrations measured during Prairie Grass experiment are used to compare observed and predicted concentrations. The paper is outlined as follows: in Section 2 we present the description of the models, in Section 3 we report the turbulence parameterization, in Section 4 we display the modelling results attained by the two semi-analytical methods and Section 5 we present the conclusions.

2. Description of the models

2.1. Eulerian model

Following Vilhena et al. [1], Moreira et al. [2], Degrazia et al. [3] and Mangia et al. [4], the steady state advection–diffusion equation is written as [6]:

$$U_i \frac{\partial C}{\partial x_i} = \frac{\partial}{\partial x_i}\left(K_i \frac{\partial C}{\partial x_i}\right), \tag{1}$$

where $i = 1, 2, 3$; C denotes the average concentration; x_i is the position; U_i is the mean wind velocity and K_i is the eddy diffusivity. The cross-wind integration of Eq. (1), in which the longitudinal axis coincides with the direction of the average wind and the longitudinal diffusion is neglected, leads to

$$U_1 \frac{\partial C_y}{\partial x_1} = \frac{\partial}{\partial x_3}\left(K_3 \frac{\partial C_y}{\partial x_3}\right), \tag{2}$$

subject to the boundary conditions of zero flux at the ground and PBL top, and a source with emission rate Q at height H_s:

$$K_3 \frac{\partial C_y}{\partial x_3} = 0 \quad \text{in } x_3 = 0, h, \tag{3}$$

$$U_1 C_y(0, x_3) = Q\delta(x_3 - H_s) \quad \text{in } x_1 = 0, \tag{4}$$

where now C_y represents the average cross-wind integrated concentration.