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Semi-analytical solution of the steady three-dimensional advection-diffusion equation in the planetary boundary layer

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Abstract

We present a three-dimensional solution of the steady-state advection-diffusion equation considering a vertically inhomogeneous planetary boundary layer (PBL). We reach this goal applying the generalized integral transform technique (GITT), a hybrid method that had solved a wide class of direct and inverse problems mainly in the area of heat transfer and fluid mechanics. The transformed problem is solved by the advection-diffusion multilayer model (ADMM) method, a semi-analytical solution based on a discretization of the PBL in sub-layers where the advection-diffusion equation is solved by the Laplace transform technique. Numerical simulations are presented and the performances of the solution are compared against field experiments data.

Keywords: Mathematical modeling; Semi-analytical solution; Advection-diffusion equation; Air pollution modeling; Planetary boundary layer

1. Introduction

Atmospheric dispersion of pollutants has attracted attention of researchers in many ways. It adds have focused on the environmental impact and health hazards; others have worked on various modeling aspects such the meteorological conditions, dispersion mechanisms, removal mechanisms, topographical features, etc. Mathematical modeling has been the case of many of these studies. The importance and the need of mathematical modeling are well known in the scientific community. There are various modeling approaches that have been used effectively in the past to deal with air pollution dispersion (Zannetti, 1990; Seinfeld and Pandis, 1998; Arya, 1999, 2003), and many of them utilize analytical approaches (Tirabassi, 1989; Lin and Hildemann, 1997; Seinfeld and Pandis, 1998; Tirabassi, 2003; Sharan et al., 2003).

In fact, the phenomenon of turbulent diffusion in the atmosphere has no single formulation, in the sense that no approach has yet been proposed having the aptness to explain all observed phenomena (Arya, 1995; Oettl et al., 2001). However, analytical solutions of equations are of fundamental importance in understanding and describing physical phenomena. Analytical solutions (as opposed to numerical ones) explicitly take into account all the

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parameters of a problem, so that their influence can be reliably investigated and it easy to obtain the asymptotic behaviour of the solution, which is usually difficult to generate through numerical calculations. Moreover, bearing in mind that the errors inherent to mathematical models are due to the modeling of the physical phenomena and numerical errors, it turns out that the analytical solutions, somehow, eliminate the numerical error of the equation solution except for the round-off error. As a consequence, becomes possible to make a more realistic analysis of the error appearing in the mathematical modeling due to the physical phenomena. In the last years (Tirabassi, 2003) special attention has been devoted to the task of searching analytical solutions for the advection-diffusion equation.

Focusing our attention in this direction, in this work we report a semi-analytical solution for the three-dimensional advection-diffusion equation in order to simulate pollutant dispersion in atmosphere considering a vertically inhomogeneous planetary boundary layer (PBL). The novelty of this work relies on the solution semi-analytically of the three-dimensional advection-diffusion equation combining the advection- diffusion multilayer model (ADMM) (Moreira et al., 2005a) and generalized integral transform technique (GITT) (Wortmann et al., 2005; Moreira et al., 2005b) methods.

The ADMM approach is based on Laplace transform technique with numerical inversion considering the PBL as a multilayer system where in each layer the eddy diffusivity and wind are constants. The main feature of this method relies on the following steps: stepwise approximation of the eddy diffusivity and wind speed, the Laplace transform application to the advection-diffusion equation, semi-analytical solution of the set of linear ordinary equation resulting for the Laplace transform application and construction of the pollutant concentration by the numerical Laplace transform inversion.

The GITT is a well-known hybrid method that had solved a wide class of direct and inverse problems mainly in the area of heat transfer and fluid mechanics (Cotta, 1993; Cotta and Mikhailov, 1997; Cheroto et al., 1999; Alves et al., 2002; Magno et al., 2002; Neto et al., 2002 and Cotta et al., 2003). The main steps of this method include the construction of the auxiliary Sturm-Liouville problem associated to the original problem, the determination of the integral transform technique in a series, using as basis the eigenfunction of the solved Sturm-Liouville problem, the replacement of this expansion in the original problem and taking moments. This procedure leads to a set of ordinary differential equation, which is classically solved by numerical methods.

Combining the ADMM and GITT methods we obtained e new technique named by us as generalized integral advection-diffusion multilayer technique (GIADMT). To reach this goal, we outline the paper as follows: in Section 2, we report the derivation of the solution for the steady three-dimensional advection-diffusion equation; in Section 3 the turbulent parameterisation assumed in this work is presented; in Section 4, the numerical results given by the new method are announced as well as the comparison with experimental data; finally, in Section 5 we present the conclusions.

2. Description of the model

The advection-diffusion equation of air pollution in the atmosphere is essentially a statement of conservation of the suspended material. The concentration turbulent fluxes are assumed to be proportional to the mean concentration gradient which is known as Fick-theory. This assumption, combined with the continuity equation, leads to the steady-state advection-diffusion equation (Blackadar, 1997)

$$u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}+w\frac{\partial c}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right)+S, \quad (1)$$

where c denotes the average concentration, K_x, K_y, K_z and u, v, w are the Cartesian components of eddy diffusivity and wind, respectively, where z is the height and S is the source term.

In order to solve the Eq. (1) we included the following assumptions: the pollutants are inert and have no additional sinks or sources downwind from the point source. The vertical (w) and lateral (v) components of the mean flow are assumed to be zero. The mean horizontal flow is Incompressible and horizontally homogeneous. Then, we have

$$u\frac{\partial c}{\partial x}=\frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\times\left(K_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right) \quad (2)$$