A NEW METHODOLOGY FOR THE SOLUTION OF THE ADVECTION-DIFFUSION EQUATION IN THE PLANETARY BOUNDARY LAYER USING CONFORMABLE DERIVATIVE

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Abstract: The objective of this work is to describe a methodological proposal for the development of a solution of the fractional two-dimensional diffusion-advection equation considering a non-homogeneous planetary boundary layer (PBL). The method ADMM (Advection-Diffusion Multilayer Method) is used, which provides a semi-analytical solution based on the discretization of the PBL in sublayers, and the advection-diffusion equation is solved by applying the Laplace transform technique, now including the novelty of the conformable derivatives. This procedure generates a new methodology called α- ADMM.

Keywords: Mathematical modeling; Advection-diffusion equation; ADMM method; Planetary Boundary Layer.

UMA NOVA METODOLOGIA PARA A SOLUÇÃO DA EQUAÇÃO DE DIFUSÃO-ADVECÇÃO NA CAMADA LIMITE PLANETÁRIA USANDO DERIVADA CONFORMÁVEL

Resumo: O objetivo deste trabalho é descrever uma proposta metodológica para o desenvolvimento de uma solução da equação difusão-advecção bidimensional fracionária, considerando uma camada limite planetária não homogênea (CLP). Utiliza-se o método ADMM (Advection-Diffusion Multilayer Method) que fornece uma solução semianalítica baseada na discretização da CLP em subcamadas e a equação de advecção-difusão é resolvida pela aplicação da técnica da transformada de Laplace, agora incluindo como novidade a derivada conformável. Este procedimento gera uma nova metodologia denominada α- ADMM.

Palavras-chave: Modelagem matemática; Equação de difusão-advecção; Método ADMM; Camada Limite Planetária.

1. INTRODUCTION

Fractional calculus has recently attracted attention worldwide for its wide range of applications in complex systems. The properties of fractional-order derivative operators generate real-world problem models with better prediction compared to modeling that apply integer-order derivatives. Mathematical modeling is a robust instrument for the development of studies in which models of natural phenomena are developed. The modeling is applied in several investigations of different aspects of meteorological conditions, dispersion mechanisms, mass and energy transport mechanisms, topographic characteristics, etc. In the atmospheric dispersion of pollutants, research focuses on environmental impacts and damage to health, standing out in the scientific community for the importance of developing and applying different mathematical models. Thus, mathematical modeling attracts the attention of researchers in the sense of applying new methodologies and techniques that more adequately represent these phenomena.

In this perspective, the objective of this work is to obtain a new methodology to simulate the behavior of the dispersion of pollutants considering the inhomogeneous turbulence in the vertical direction, applying the ADMM (Advection-Diffusion Multilayer Method) methodology [1,2]. The novelty of the present work is that the combination of this methodology with the conformable derivatives results in a new methodology to study the atmospheric dispersion process [3]. The ADMM approach applies the Laplace transform technique with numerical inversion and considers PBL as a multilayer system in which each layer the diffusivity of the eddies and the wind are constant. The main characteristic of this method is based on the following steps: step-by-step approximation of turbulent diffusivity and wind speed, application of the Laplace transforms to the diffusion-advection equation, semi-analytical solution of the set of ordinary linear equations obtained from the application of Laplace transform and construction of pollutant concentration by numerical inversion of Laplace transform.

2. METHODOLOGY

The conformable derivative represents a new and simple definition of a fractional derivative [4,5]. This new definition turns out to be a natural extension of the usual derivative and satisfies practically all the specifics of integer-order derivatives, thus meeting, for example, properties such as the derivative of the product and the quotient of two functions, and the chain rule. Since the other definitions of fractional derivatives do not satisfy these properties.

So, if *f* diferenciável differentiable, then,

$$T_\alpha = [\, f(x)] = x^{1-\alpha} \frac{df(x)}{dx} \tag{1}$$

where T_α represents the conformable derivative [3].

The fractional diffusion-advection equation can be written as follows:

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$$u(z)\frac{\partial^{\alpha} c(x,z)}{\partial x^{\alpha}} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial c(x,z)}{\partial z}\right) \quad , \quad 0<\alpha\leq 1 \tag{2}$$

Normally, linear integer-order equations are simpler to obtain the solution. However, results obtained in recent works with validated simulations in line with experiments widely known in the literature are the motivation to apply the conformable operator in this work [7,8,9,10].

Thus, introducing Eq. (1) into (2), results:

$$u(z)x^{1-\alpha}\frac{\partial c(x,z)}{\partial x} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial c(x,z)}{\partial z}\right) \quad , \quad 0<\alpha\leq 1 \tag{3}$$

It is observed that the structure of equations (2) and (3) was modified through the insertion of fractional order parameters. This procedure, from a physical point of view, causes dimensional inconsistency in the solution, requiring dimensional corrections in the fractional equation. Then, a parameter is inserted that allows correcting the dimension of the physical quantities present in the equation. Thus, the procedure adopted in the work of Gomez-Aguilar [11] is adopted, where an auxiliary factor is introduced $\phi^{1-\alpha}$ in equation (3).

$$u(z)\left(\frac{x^{1-\alpha}}{\phi^{1-\alpha}}\right)\frac{\partial c(x,z)}{\partial x} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial c(x,z)}{\partial z}\right) \quad , \quad 0<\alpha\leq 1 \tag{4}$$

The equation (4) allows to improve the understanding of the dispersion process of air pollutants with application of the fractional derivative in the advective term and with a semi-analytical solution to be obtained from the combination of the conformable derivative with the ADMM method [1,2].

2.1 The ADMM method

To solve Eq. (4), the ADMM method is used [12], which consists of dividing the PBL (Planetary Boundary Layer) into sublayers so that the fractional advection-diffusion equation has dependence on the variable *z*. Figure 1 show schematically the subdomain of the variable *z*, where the layer in which there is emission of pollutants is denoted by *n**.

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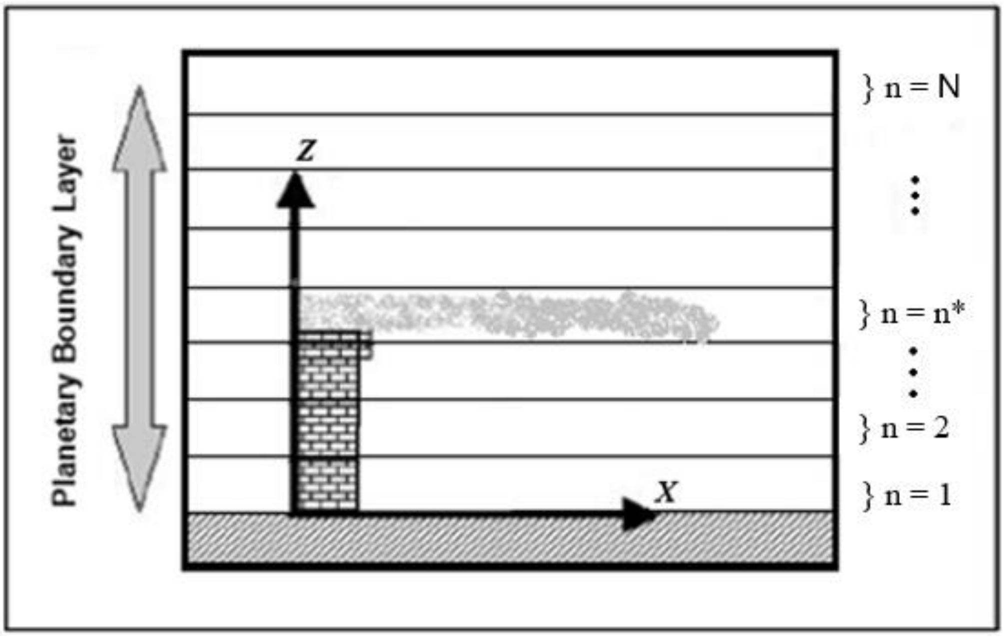
Figure 1. Schematic representation of the ADMM model [2]



In each sublayer, a stepwise approximation is taken, in which the average values of the parameters that depend on height are considered, such as the eddy diffusivities and the wind speed profile. Thus, N similar problems are obtained, coupled by conditions of concentration and flow continuity interfaces. In this way, Eq. (4) can be rewritten as a multilayer system:

$$\bar{u}_n \frac{\partial c(X,z)}{\partial X} = \bar{K}_n \frac{\partial^2 c(X,z)}{\partial z^2} \quad , \quad 0 < \alpha \le 1 \tag{5}$$

with $z_n \le z \le z_{n+1}$, $X > 0$; $n = 1,2,3,...N$, where N is the number of sublayers in which the PBL was divided and c_n is the concentration at the n[th] layer. Note that a variable change was made,

$$X = \phi^{1-\alpha} \int_0^x x^{\alpha-1} dx \tag{6}$$

Following the ADMM methodology, to account for the vertically inhomogeneous turbulence (which is dependent on z), continuity conditions are imposed for the concentration and concentration flux at the interfaces:

$$c_n = c_{n+1}$$

$$\bar{K}_n \frac{\partial c_n}{\partial z} = \bar{K}_{n+1} \frac{\partial c_{n+1}}{\partial z}$$

where $n = 1,2,...(N-1)$. In this way, N problems arise that are interconnected by the conditions of the continuity of the concentration and flux, where $\bar{K}_n$ and $\bar{u}_n$ assume a constant average value in each sublayer.

For the solution of Eq. (5), it is necessary to specify the source and boundary conditions. In this way, the following source condition is considered:

$$c(0,z) = \frac{Q}{\bar{u}} \delta(z - H_s) \tag{7a}$$

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where Q is the emission rate, δ is the Dirac delta function and H_s is the height of the source. In addition, the following boundary conditions are imposed:

$$\bar{K}\frac{\partial c}{\partial z} = 0 \quad , \quad z = h \tag{7b}$$

$$\bar{K}\frac{\partial c}{\partial z} = v_d\, c \quad , \quad z = z_o \tag{7c}$$

where v_d is the deposition velocity of the gaseous pollutant. It is selected the lower boundary condition at z_o, the roughness length, the height corresponding to that at which a deposition velocity may have been measured (typical value of z_o is 1 m).

By applying the Laplace transform to the variable X in Eq. (5) results:

$$\frac{\partial^2 \hat{c}_n(s,z)}{\partial z^2} - \left(\frac{\bar{u}_n s}{\bar{K}_n}\right)\hat{c}_n(s,z) = -\frac{Q}{\bar{K}_n}\delta(z - H_s) \tag{8}$$

and the solution is given by:

$$\hat{c}_n(s,z) = g_{1n}e^{T_1^n z} + g_{2n}e^{T_2^n z} + \frac{Q}{T_3^n}\left[e^{T_1^n(z-H_s)} - e^{T_2^n(z-H_s)}\right] \tag{9}$$

where

$$T_1^n = \left(\frac{\bar{u}_n s}{\bar{K}_n}\right)^{1/2} \;;\; T_2^n = -\left(\frac{\bar{u}_n s}{\bar{K}_n}\right)^{1/2} \;;\; \text{and } T_3^n = 2\left[\bar{K}_n \bar{u}_n s\right]^{1/2}$$

and g_{1n} and g_{2n} are the constants resulting from the resolution of the linear system due to the boundary and interface conditions.

Finally, in Eq. (9) it is necessary to apply a Laplace transform inversion method. In this work, the inversion will be performed through the Fixed Talbot (FT) algorithm [13], thus resulting in Eq. (10):

$$c_n(x,z) = \frac{r}{M}\left\{\frac{1}{2}c_n(r,z)e^{rx} + \sum_{k=1}^{M-1}\mathrm{Re}\left[e^{xs(\theta_k)}\hat{c}_n(s(\theta_k),\mathrm{z})(1 + \mathrm{i}\,\tau(\theta_k))\right]\right\} \tag{10}$$

where

$$s(\theta_j) = r\theta(\cot\theta + 1), -\pi < \theta < +\pi$$

$$\tau(\theta_j) = \theta_j + (\theta_j \cot\theta - 1)\cot\theta_k$$

$$\theta_j = \frac{k\pi}{M}$$

Here, r is a parameter based on numerical experiments and M is the number of terms in the summation in the FT algorithm. For more details, see the work [14].

3. CONCLUSION

The main objective of this work was to describe a new methodology called α-ADMM to obtain a solution of the fractional two-dimensional diffusion-advection equation, considering a non-homogeneous PBL. In this proposal, the ADMM method is used, which provides a semi-analytical solution based on the discretization of PBL in sublayers, and the advection-diffusion equation is solved by applying the Laplace transform technique, standing out as a novelty the inclusion of the conformable derivative. The next steps consist of using the obtained solution to simulate the dispersion of pollutants in the atmosphere in physical situations related to atmospheric stability and soil deposition problems. Expected through the α-ADMM methodology to obtain a better description of the diffusion process of atmospheric pollutants.

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