AN ANALYTICAL SOLUTION FOR THE DISPERSION EQUATION OF ATMOSPHERIC POLLUTANTS WITH FRACTIONAL PARAMETER IN THE DIFFUSIVE TERM USING CONFORMABLE DERIVATIVE

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Abstract:

This study aims to investigate the potential of fractional derivatives in atmospheric dispersion modeling. Therefore, an analytical solution of the two-dimensional fractional advection-diffusion equation is proposed using GILTT and conformable derivatives methods. The novelty of this study is the insertion of a fractional parameter in the diffusive term considering the conformable derivative, considering the anomalous behavior in the diffusion process, resulting in a new methodology here called α-GILTT method. The simulations were compared with the moderately unstable data from the Copenhagen experiment and the best results are for the fractional parameter α = 0.99.

Keywords: α-GILTT, Anomalous diffusion, Conformable derivatives.

Resumo: Este estudo tem como objetivo investigar o potencial de derivados fracionários na modelagem de dispersão atmosférica. Portanto, uma solução analítica da equação bidimensional de advecção-difusão fracionada é proposta usando métodos GILTT e derivados conformáveis. A novidade deste estudo é a inserção de um parâmetro fracionário no termo difusivo considerando a derivada conformável, levando em consideração o comportamento anômalo no processo de difusão, resultando em uma nova metodologia aqui denominada método α-GILTT. As simulações foram comparadas com os dados moderadamente instáveis do experimento de Copenhagen e os melhores resultados são para o parâmetro fracionário α = 0.99.

Palavras-chave: α-GILTT, Difusão anômala, Derivada conformável.

INTRODUCTION

Anomalous diffusion is present in a wide variety of experimental scenarios in physics, chemistry, biology, and other branches of engineering, being an expanding field of research that has attracted a lot of attention from the scientific community. An important application of anomalous diffusion is related to the description of turbulent diffusion in the atmosphere. The pioneer in understanding this phenomenon was Richardson [1], who, based on his observations, concluded that the increase in the width of the plumes of pollutants emitted by point sources occurred in the proportion of t^{β}, with $\beta \geq 3$, inconsistent with the typical diffusion, where there are $\beta = 1$. Although turbulent diffusion is often modeled using the classical (integer-order) advection-diffusion equation, this type of approach has proved ineffective in describing the anomalous diffusion caused by turbulence [2].

In recent years, fractional calculus has proven to be the most adequate mathematical theory to deal with the complexity of anomalous diffusion, as described in articles [3-6]. Although they are linear operators, fractional derivatives do not have the same operational properties as Newton's derivative, such as the product rule, quotient rule, and chain rule. The absence of these properties in the fractional calculation causes a series of obstacles in the mathematical handling of models, often leading to the need for complex numerical methods. These inconveniences have led to the development of the local fractional derivative, which enjoys most of the properties of the integer-order derivative [7-10].

This article aims to investigate the potential of conformable derivative in modeling the dispersion of air pollutants and in the description of anomalous diffusion. For this, an analytical solution of the fractional, two-dimensional, and stationary diffusion-advection equation is proposed, using the GILTT (Generalized Integral Laplace Transform Technique) [11-19] and conformable derivatives methods [9]. The novelty of this study is the insertion of a fractional parameter in the diffusive term, together with the conformable derivatives, considering the anomalous and non-differentiable behavior of the problem, resulting in a new methodology here called the α-GILTT method.

It should be noted that the analytical solution of the diffusion-advection equation proposed in this work, considering a fractional parameter in the diffusive term and variable coefficients, has no known solution in the literature. The proposed model was solved and compared with data from the Copenhagen experiment, which are considered to have moderately unstable atmospheric stability.

2. METHODOLOGY

To apply the α-GILTT method, the classical two-dimensional fractional advection-diffusion equation is modified by inserting fractional operators in the diffusive term, obtaining:

$$u(z)\frac{\partial c(x,z)}{\partial x} = \frac{\partial^{\alpha}}{\partial z^{\alpha}}\left(K_z(z)\frac{\partial^{\alpha} c(x,z)}{\partial z^{\alpha}}\right) \quad , \quad 0 < \alpha \le 1 \tag{1.1}$$

where $u(z)$ is the vertical profile of the wind speed in the longitudinal direction, $c(x,z)$ is the mean concentration of the passive contaminant, and $K_z(z)$ is the coefficient of vertical diffusion. In the direction of the spatial coordinate z, the boundary conditions are zero flux on the ground and at the height of the planetary boundary layer (PBL), and the source condition is given by

$$c(0,z) = \frac{Q}{U(z)}\delta(z - h_s) \tag{1.2}$$

where Q is the source intensity, h_s is the source height, and δ is the delta-Dirac function.

To correct the dimensionality of the proposed model, the suggestion provided in the work [20] was adopted, introducing an auxiliary factor φ [21] in equation (2.1):

$$\frac{d}{dz} \to \frac{1}{\varphi^{1-\alpha}}\frac{d^{\alpha}}{dz^{\alpha}} \tag{1.3}$$

Relation (2.3) is valid if the parameter φ has a length dimension [L]. Thus, the fractional representation of Eq. (2.1), to be solved in this work, is given by:

$$u(z)\frac{\partial c(x,z)}{\partial x} = \frac{1}{\varphi^{2(1-\alpha)}}\frac{\partial^{\alpha}}{\partial z^{\alpha}}\left(K_z(z)\frac{\partial^{\alpha} c(x,z)}{\partial z^{\alpha}}\right) \quad , \quad 0 < \alpha \le 1 \tag{1.4}$$

The conformable derivative method [9] is given by:

$$T_\alpha\left[f(z)\right]=z^{1-\alpha}\frac{df(z)}{dz} \qquad (1.5)$$

Thus, the first step is to apply to the diffusive term of equation (2.4) the relation (2.5):

$$u(z)\frac{\partial c(x,z)}{\partial x}=z^{1-\beta}\frac{\partial}{\partial z}\left[K_z(z)\left(\frac{z}{\varphi^2}\right)^{1-\beta}\frac{\partial c(x,z)}{\partial z}\right] \qquad (2.6)$$

To obtain a more general solution of Eq. (2.6), the following equality will be considered:

$$F(z)=K_z(z)\left(\frac{z}{\varphi^2}\right)^{1-\beta} \qquad (2.7)$$

thus, by substituting Eq. (2.7) in Eq. (2.6), we obtain:

$$u(z)\frac{\partial c(x,z)}{\partial x}=z^{1-\beta}\frac{\partial}{\partial z}\left[F(z)\frac{\partial c(x,z)}{\partial z}\right] \qquad (2.8)$$

Applying the chain rule to the diffusive term of Eq. (2.8) [11], and inserting the necessary simplifications, we obtain the equation of the auxiliary problem:

$$\psi_i''(z)+\lambda_i^2\psi_i(z)=0 \quad , \quad 0<z<h \qquad (2.9)$$

$$\psi_i'(z)=0 \quad , \quad z=0,h \qquad (2.10)$$

and this problem has the traditional solution given by:

$$\psi_i(z)=\cos(\lambda_i z) \quad , \quad \lambda_i=\frac{i\pi}{h} \quad , \quad i=0,1,2,... \qquad (2.11)$$

The next step is to expand the concentration $c(x,z)$ into a series, the final solution being:

$$c(x,z)=\sum_{i=0}^{\infty}\frac{A_i(x)\psi_i(z)}{\sqrt{N_i}} \qquad (2.12)$$

where $A_i(x)$, with *n* = 0, 1, 2, ... being the unknown coefficients of the series, and *N* the norm.

We apply Eq. (2.12) in Eq. (2.8) to determine the coefficients $A_i(x)$ and then multiply by the integral operator $\frac{1}{\sqrt{N_j}}\int_0^h \psi_j(z)dz$, obtaining:

$$\sum_{i=0}^{\infty}\left(\int_0^h u(z)\frac{\psi_j(z)\psi_i(z)}{\sqrt{N_j}\sqrt{N_i}}dz\right)\frac{\partial A_i(x)}{\partial x}=$$

$$\sum_{i=0}^{\infty}\left[\int_0^h \frac{\psi_j(z)}{\sqrt{N_j}}\left\{z^{1-\beta}F'(z)\frac{\frac{\partial \psi_i(z)}{\partial z}}{\sqrt{N_i}}-z^{1-\beta}\lambda^2 F(z)\frac{\psi_i(z)}{\sqrt{N_i}}\right\}dz\right]A_i(x) \qquad (2.13)$$

Rewriting Eq. (2.13) in matrix form, we have:

$$A'(x)+GA(x)=0 \qquad (2.14)$$

where $A(x)$ represents a vector, *G* is the matrix $G=B^{-1}E$ and, $A(0)=A_0$, the initial condition.

The initial condition is obtained by applying the same procedure to expand $c(x,z)$. Next, Eq. (2.14) is then solved by applying the Laplace transform and the diagonalization process [23], providing the following transformed solution:

$$\overline{A(s)}=W\left(s.I+D\right)^{-1}W^{-1}.A(0) \qquad (2.15)$$

Applying the inverse Laplace transform to Eq. (2.15), we have:

$$A(x)=W.L^{-1}\left\{\left(s.I+D\right)^{-1}\right\}W^{-1}.A(0) \qquad (2.16)$$

where *D* represents the diagonal matrix of eigenvalues, *W* the matrix of the eigenfunctions of *G*, W^{-1} its inverse and *I* represent the identity matrix.

The elements of the matrix $(sI+D)$ have the form $\{s+d_i\}$, where d_i being the eigenvalues of the matrix *G* or the elements of the diagonal matrix *D*. As $(sI+D)$ being a diagonal matrix, in matrix algebra its inverse is given by the multiplicative inverse of the main diagonal elements. Thus, the elements of the matrix $(sI+D)^{-1}$ take the form $\frac{1}{s+d_i}$, whose inverse Laplace transform is e^{-xd_i} .

Thus, the solution of the problem proposed by equation (2.4) is finally obtained and given by Eq. (2.12).

3. RESULTS AND DISCUSSIONS

The data presented in this section were generated from meteorological information from the Copenhagen experiments [24]. The model was parameterized with the vertical diffusion coefficient proposed by Degrazia [25], logarithmic wind profile, and for simplicity, correction of the dimensionality $\varphi = 1$ m.

Table I displays the statistical indices generated by the model considering different values of the fractional parameter. The model performance was statistically evaluated using the bootstrap procedure described by Hanna (1989) and the following metrics:

Normalized mean square error (NMSE) =$\overline{(C_o - C_p)^2} / \overline{C_p}\,\overline{C_o}$,

FAT2 = fraction of data for which $0.5 \leq (C_p/C_o) \leq 2$,

Correlation coefficient (COR) = $\overline{(C_o - \overline{C_o})(C_p - \overline{C_p})} / \sigma_o \sigma_p$,

Fractional bias (FB) = $\overline{C_o} - \overline{C_p} / 0.5(\overline{C_o} + \overline{C_p})$,

Fractional standard deviation (FS) = $(\sigma_o - \sigma_p)/0.5(\sigma_o + \sigma_p)$,

where the subscripts o and p refer to the observed and predicted quantities, respectively, and the overbars indicate average values. The FB reflects whether the expected quantities underestimate or overestimate the observed values. The NMSE represents the dispersion of the model output in relation to the dispersion of the data. The best results are expected to give values close to zero for the NMSE, FB, and FS and close to 1 for COR and FAT2.

Taking as reference the observed statistical indices for $\alpha = 1$ (integer-order advection-diffusion equation), the best indicators were obtained with $\alpha = 0.99$. Although the parameters Nmse, Cor, and Fa2 are relatively close for the two simulations, it is observed that the Fb and Fs indicators are better for $\alpha = 1$. It should be noted that this experiment has moderately unstable atmospheric stability, and values very close to one are expected for the fractional parameters (low fractionality). Effectively, the fractional parameter for this experiment, comparing the results for $\alpha = 0.99$ and $\alpha = 1$ are statistically very similar.

Table I. Model statistical indices using data from the Copenhagen experiment.

Case	α	Nmse	Cor	Fa2	Fb	Fs
I	1.00	0.08	0,91	1.00	0.11	0.29
II	0.99	0.10	0.91	1.00	0.17	0.32
III	0.98	0.13	0.91	1.00	0.22	0.35
IV	0.97	0.17	0.91	1.00	0,28	0.39

4. CONCLUSION

The present work proposes a new methodology to obtain the solution of the fractional advection-diffusion equation based on the GILTT methods and conformable derivatives. This methodology allows using a diffusion coefficient that depends on the z variable, thus considering the inhomogeneity of turbulence in the vertical direction. Although the result with the whole order fractional parameter presented the best result, considering the data from the Copenhagen experiment, the influence of this parameter in the simulations was clearly observed. The next step of the research will be to insert fractional parameters in all derivatives of the equation, submitting the model to strongly convective (very unstable) atmospheric conditions, using data from the Prairie Grass experiment.

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5. REFERENCES

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