A three-dimensional fractional solution for air contaminants dispersal in the planetary boundary layer

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ABSTRACT

In this study, we investigated some closed-form solutions for solving atmospheric dispersion issues under variable atmospheric hypothesis, in a vertically positioned non-homogeneous planetary boundary-layer. In our context, a nonidentical expansion for the solution of the fractional advection-diffusion equation in a non-integer dimensional-space was examined. In a nutshell, a Sturm-Liouville eigenvalue problem with more reliable information concerning the initial value problem is discussed. The performance of the model was estimated by presenting numerical simulations against experimental data. Under these meteorological conditions, fractional-order models performed far better than those of the classical integer-order ones.

1. Introduction

Considering, the advantage of a familiar classical solution of the stationary problem with advection previously developed [1, 2], effort have been made over the years to obtain analytical solutions of the same equation in order to model air pollution. Nowadays, we noted a solid attention in analytical solutions of differential equations, in which some integro-differential operators, particularly fractional differential equations, have been widely explored to characterise many environmental transport phenomena [3, 4, 5]. The fractional equations we consider and their practical applications turn out to be tremendously a convenient tool to investigate anomalous diffusion [6, 7, 8, 9]. Atmospheric pollution no matter its origin has been consistently and methodically simulated by conventional differential equations in integer order dimensions space [10, 11, 12]. However, there is a gap between classical analytical solutions and fractional order derivative solutions concerning atmospheric pollutants dispersion, in the case of modeling turbulent diffusion. This problem is due to the non-differentiable behaviour of the transport process and the presence of anomalous diffusion [13, 14]. In fact, turbulence provides the real explanation for the dispersion of contaminants in the biosphere, given that the turbulent flow in the pollution models is directed after the field lines of mean wind speeds; showing slightest diffusion in a different orientation. Anomalous diffusion processes are found in various complex systems, with characteristic being the non-linear expansion of the mean squared displacement as time goes by. On the contrary, traditional diffusion often follows Gaussian statistics, and therefore Fick’s second law collapses to outline the connected transport response. Often, deviations are observed from the linear time reliance of the mean squared displacement, which mean that the anomalous diffusion behaviour is well-tight connected with the failure of the central limit theorem, resulting to random distributions or long-range correlations. Today, anomalous diffusion is linked to the Lévy-Gnedenko generalised central limit theorem. In such cases, not all moments exist [15, 16]. Fractional diffusion is non-universal, i.e. entails a parameter α determining the fractional derivative order. The α parameter is used to determine the domains or sub-domains of anomalous diffusion. Our interest in this study will be focused on the description of sub-diffusive phenomena, which correspond to the $0 < \alpha < 1$ interval. In the PBL, when a plume is dispersed, the evolution of its shape and internal structure is determined by the interaction between the plume and the turbulent eddies that characterize atmospheric motion. This result is quite similar regardless of current advances in the theory and numerical simulation of turbulent dispersion in the PBL. The need for a fast and flexible method to predict the transport of pollutants and other contaminants derived from distributed surface sources in the atmosphere remains highly critical [17]. The advection-diffusion equation has for a long time utilised to report air contaminants dispersion in the turbulent atmosphere [18]. For instance, the classical air pollution model assumes
wind speed and eddy diffusivity as constants in the PBL [19]. Therefore, over-time, the idea of wind speed and eddy diffusivity considered as constant have been tempered to find more reliable solutions of the advection-diffusion equation. Hence, some works researched attempts to obtain the analytical solutions of the two or three dimensional steady-state advection-diffusion equation, depicting the crosswind integrated concentrations in the atmosphere, for precise wind speed and vertical eddy diffusivity [20, 21, 22, 23]. However, nearly all the crosswind-integrated solutions are got by supposing the wind speed and vertical eddy diffusivity like the power-law functions of vertical height above the ground, in conditions of horizontally homogeneous turbulence in the PBL [24]. Nevertheless, these wind speed and eddy diffusivity profiles may not simulate processes that happens in the PBL in a realistic manner due to its complex turbulent structure under various stability conditions. To overcome the limited efficiency of analytical transport solutions with peculiar shapes of wind speed and vertical eddy diffusivity, the use of fractional models seems appropriate by underlining the non-conservative aspect of most real-world phenomena. In addition, to deal with the turbulent dispersion of a pollutant discharged by a continuous source in the PBL; the anomalous diffusion approach, assumed that the physical structure of turbulence and velocity fields are outlined by complex physical features: diffusion coefficient and mean velocity profile that are identified together as functions of spatial reference systems. These functions are often chosen with a view to fit experimental data, otherwise obtained from Taylor statistical diffusion theory [25, 26]. As such, in order to investigate the capability of the application of fractional operators to modeling dispersion of pollutants in the atmosphere, we put forward a fractional differential equation model for the spatial distribution of concentration of air pollutants in Planetary Boundary Layer (PBL). We solve the model and compare the solutions with conventional integer order derivative model against a real experiment.

The paper is sequenced as follows: Sections 2 and 3 review the fractional order derivative. The mathematical model is presented and resolved analytically in Section 4. Numerical comparison of our solution against integer order derivative model and experimental data is done in Sections 5 and 6. Section 7 presents the conclusions.

2. A note on fractional order derivatives

It is well-known that the standard mathematical models of integer order derivatives, including nonlinear models, do not work properly in many experiments [27, 28]. To overcome this problem, the concept of fractional order derivatives for a function has been inspired by L'Hospital (1695) which polished meaning of Leibniz’s currently most useful notation \( \frac{dy}{dx} \) for derivative of order \( n \in \mathbb{N}_0 := 0, 1, 2, \ldots \) with \( n = \frac{1}{2} \). Therefore, L’Hospital, Euler, Lagrange, Laplace, Riemann and Liouville developed the basic concept of fractional calculus [29, 30, 31, 32]. In this regard, fractional order derivatives for a given function \( f(x) \), are well-established in the generalisation of the Abel integral:

\[
D^{-α} f(x) = \frac{1}{\Gamma(α)} \int_0^x (x-r)^{α-1} f(r) dr,
\]

where \( n \) is a nonzero positive integer and \( \Gamma(\cdot) \) represents the Gamma function [33]. This embodies an integral of order \( n \) for the continuous function \( f(x) \), at any time \( f \) and all its derivatives vanish at the origin, \( x = 0 \). This outcome can be expanded to the idea of an integral of arbitrary order \( α \), defined as:

\[
D^{-α} f(x) = D^{-β}_{-α} f(x) = \frac{1}{\Gamma(α)} \int_0^x (x-r)^{α-1} f(r) dr,
\]

where \( α \) represents a positive real number and an integer such that \( 0 < α \leq 1 \).

Let’s assume that \( i \) is the positive integer sizeable than \( α \), so that \( α = m − β, 0 < β \leq 1 \). Equation (1) could be introduced to describe the derivative of (positive) fractional order, so-called \( α \), of a function \( f(x) \) as:

\[
D^α f(x) = D^{−β}_{−α} f(x) = \frac{1}{\Gamma(β)} \int_0^x f(x) dr.
\]

It is worth noting that these solutions, like Abel’s integral, are simply well founded when depending on the condition that \( f^{[k]}(x)|_{x=0} = 0 \) for \( k = 0, 1, 2, \ldots, β \) [34].

Take the advantage of the usual classical fractional integrals and derivatives, we refer to the definition of Caputo and Riemann-Liouville derivative integrals. Thus, for a function \( f \) outlined in an interval \( I = [a, b] \), the Riemann-Liouville integrals \( J_{a^+}^α f \) and \( J_{b^-}^α f \) of order \( α \in C(Re(α) > 0) \) are clarified respectively by [35]

\[
\begin{align*}
(J_{a^+}^α f)(t) &= \frac{1}{\Gamma(α)} \int_a^t f(s) ds, \\
(J_{b^-}^α f)(t) &= \frac{1}{\Gamma(α)} \int_t^b f(s) ds.
\end{align*}
\]

Where \( \Gamma(α) \) represents the usual Gamma function. In this context, the left and right Riemann-Liouville fractional derivatives \( (D^α_{a^+} f)(t) \) and \( (D^α_{b^-} f)(t) \) are:

\[
\begin{align*}
(D^α_{a^+} f)(t) &= \frac{1}{\Gamma(n-α)} \int_a^t f^{(n)}(s) ds, \\
(D^α_{b^-} f)(t) &= \frac{(-1)^n}{\Gamma(n-α)} \int_t^b f^{(n)}(s) ds.
\end{align*}
\]

3. Properties

1. [36]

If \( Re(α) > 0 \) and \( β \in C(Re(β) > 0) \),

\[
\begin{align*}
(D^α_{a^+} f)(x) &= \left(J_{a^+}^α f\right)(x), \\\n(D^α_{b^-} f)(x) &= \left(J_{b^-}^α f\right)(x)
\end{align*}
\]

are verified on almost all points \( x \in [a, b] \) for \( f \in Lp(a, b), (1 \leq p \leq \infty) \). If \( α > β > 1 \), then the aforementioned relations hold at any point of \([a, b].\)

2. The juncture between Caputo fractional derivative and Riemann-Liouville fractional derivative is given by the following formula [37].

\[
\frac{D^α_{a^+} f}{\Gamma(1 - α)} x^{-α}. \]

4. Mathematical description

Let’s consider the spatial distribution \( \bar{z} = \bar{z}(x, y, z) \) of a contaminant rejected from a source in the PBL relied on K-theory [38].
\[
\frac{\partial \sigma}{\partial t} - \frac{\partial}{\partial x} \left( k_x \frac{\partial \sigma}{\partial x} \right) + \frac{\partial}{\partial y} \left( k_y \frac{\partial \sigma}{\partial y} \right) + \frac{\partial}{\partial z} \left( k_z \frac{\partial \sigma}{\partial z} \right) = 0.
\]

(11)

where \( \sigma \) is the average concentration, \( u \) and \( k_x, k_y, k_z \) are the Cartesian elements of wind velocity and eddy diffusivities along the \( x, y \) and \( z \)-directions, respectively. The ensuing assumptions are considered under moderate to strong wind conditions, thus the diffusion term in the \( x \)-direction is slightly less than the advection term. In addition, eddy diffusivities are represented by the following expressions:

\[
K_x(x, z) = f_1(x)u(z), \quad K_y(x, z) = f_2(x)K_z,
\]

(12)

where \( f(x) \) depends on \( x \) call attention to correction of \( K_y \) in the vicinity of the source, and \( K_z \) stands for the distant-field eddy diffusivity which depends on \( z \). The three-dimensional concentration stems from Glénio et al. (2018) [39] using the variable separations method can be deduced from Equation (11) by taking into account \( f(x) = \frac{1}{2} \frac{\partial}{\partial x} \sigma^2(x) \) and \( f_y(x) = \frac{1}{2} \frac{\partial}{\partial y} \sigma^2(x) \), where \( \sigma_x \) and \( \sigma_y \) are dispersion coefficients in the \( y \) and \( z \)-directions respectively. The functional form of \( K_z \) is sketched out to allow Gaussian distribution for the transverse concentration. In agreement with these considerations, Equation (11) becomes:

\[
\frac{d \sigma}{d t} + \frac{\partial}{\partial x} \left( K_x \frac{\partial \sigma}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial \sigma}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_z \frac{\partial \sigma}{\partial z} \right) = 0.
\]

(13)

When the process is driven by the steady state regime of the transport equation with \( K_z \) constant training in the domain a sharp boundary condition \( \tau_z(0, z) = \lim_{x \to \infty} \tau_z(x, z) = \delta(z), 0 < \infty < \infty \), and \( -\infty < \infty < \infty \), the underneath solution follows Brownian distribution given by the Galilei shifted Gaussian. It is well-known that the advantage of the random walk models, using the fractal approach could be feasible to insert external fields in a direct way. Thus, considering transport in phase space extended by the both position and velocity coordinates. However, the assessment of the boundary value problems seems analogous to classical equations [40].

\[
\tau_z(x, z) = \frac{1}{\sqrt{4\pi K_x} \cdot \alpha} \exp \left( -\frac{x^2}{4\alpha^2 K_x} \right).
\]

(14)

By introducing the well-known scaling rules for the Fourier and Laplace transforms, Equation (15) below is obtained:

\[
f(\alpha) \Psi(\alpha) = f(k), \quad a \in \mathbb{R}, f(bf)\Psi.
\]

(15)

As reported by [41], a tridimensional solution, for ground level sources is proposed. Thus, a modified CTRW scheme introduced, and applied to an extended Taylor, assuming the initial condition \( \tau_z(x, 0) = \delta(x) \). The resulting equation in Fourier-Laplace space becomes:

\[
\frac{\partial \sigma_k}{\partial \alpha} = -x^2 K_x \tau_k(x, s) - x^2 K_z \tau_z(x, s) = \frac{\partial}{\partial x} \left( \frac{k_x}{k_z} \tau_k(x, s) \right).
\]

(16)

Supposing a waiting time distribution, especially for the range of a long-tailed distribution for \( \Psi, \psi(u) \sim 1 - \frac{1}{u^\gamma} \) for \( u \to 0 \) and \( k \to 0 \), in the asymptotic shapes \( \lambda_x(k) \sim 1 - \alpha \sigma^2 [k] \) for the cosine transformation, after a tricky development. We have a situation where the Laplace transform of the sticking probability is:

\[
\phi(k, u) = \frac{1 - \Psi(u)}{u} - \frac{\partial}{\partial \sigma} \psi(u),
\]

(18)

and the term \( \left[ \frac{1 - \Psi(u)}{u} \right] \) stand for the Laplace transformed sticking probability

\[
\Phi(t) = 1 - \int_0^t dt' \psi(t').
\]

(19)

Accordingly to Weiss treatise [42], in the Fourier-Laplace space

\[
U \phi_x(k, a) - \phi_x(k, 0) = \frac{U \Psi(u) \psi(k) \phi_x(k, a) - \psi(u) \phi_x(k, 0)}{u},
\]

(20)

the Fourier transform \( \phi(k) \) corresponds to operator in \( k \) thus,

\[
\phi(k) \varepsilon_x(k, x) \equiv \lambda_x(k) \varepsilon_x(k, x).
\]

(21)

Assuming that sub-diffusion is symbolised by finite transfer variance \( \Sigma^2 \), for small \( k \), the following relation is obtained

\[
\varepsilon_x(k, u) - \varepsilon_x(k, 0) = u^{-a} L(y, x) \varepsilon_x(k, u).
\]

(22)

Using the Riemann-Liouville fractional differentiation definition of order \( 1 - a \), it is obtained

\[
\alpha D_x^{1-a} \varepsilon_x(k, u) \equiv \frac{\partial}{\partial x} \int_0^x \varepsilon_x(k, x') \frac{x}{(x-x')^{1-a}} dx'.
\]

(23)

By integrating the corresponding formula

\[
\alpha D_x^{1-a} \{ \alpha D_x^{1-a} \varepsilon_x(k, x) \} = u^{-a} \varepsilon_x(k, u),
\]

(24)

the following fractional partial equation is derived

\[
\frac{\partial \varepsilon_x(k, u)}{\partial x} = 0, \quad \alpha D_x^{1-a} L(y, z) \varepsilon_x(k, u).
\]

(25)

introducing the operator \( L(y, z) = \frac{\partial}{\partial z} [K_y \frac{\partial}{\partial y} K_z] + K_z \frac{\partial^2}{\partial y^2} \).

By choosing our solution in the ansatz form

\[
\varepsilon_x(y, z) = X_x(Y_x)(y)Z_z(z).
\]

(26)

The resulting equation is

\[
\frac{d Y}{d x} \left( \alpha D_x^{1-a} X \right) = \frac{L(y, z)Y^2}{Z^2}.
\]

(27)

is then split into the pair of eigen-equations [43].

\[
\alpha D_x^{1-a} X(x) = \frac{x^a \delta(0)}{1 - a} = Y(z).
\]

(28)

For an eigenvalue \( \lambda_{x,a} \) of \( L(y, z) \) and \( u = 1 \) for simplification. We found, the fractional generalized diffusion equation:

\[
\frac{\partial^2 \tau_x(y, z)}{\partial x^a} = \frac{x^a \delta(y)}{1 - a} + K_y \frac{\partial^2 \tau_x(y, z)}{\partial y^2}.
\]

(29)

Finally, for Equation (29) to describe a practical real problem of dispersion in Planetary Boundary Layer (PBL), it should be subject to boundary conditions.

\[
K_z \frac{\partial}{\partial z} \tau_z(y, z) = 0, \quad z = z_0, \quad z = h.
\]

(30)

\[
\tau_x(0, y, z) = 0, \quad \tau_x(z, 0, z) = \delta(z - H_x \delta(0)), \quad x = 0.
\]

(31)

where \( z_0 \) symbolises the surface roughness length, \( h \) represents PBL height and \( \delta(\cdot) \) stands for Dirac delta function. The pollutant is released from an elevated source point emission rate \( Q \) at height \( H_x \), with the equivalence of zero flux i.e. ground \((z = z_0)\) and top \((z = h)\).

The solution is obtained by using the corresponding ansatz [44].

\[
\tau_x(y, z) = \sum_{n=0}^N X_x(n)a_n(y, z).
\]

(32)

This generates the two ordinary differential equations.

\[
\frac{\partial X}{\partial x} - \frac{x}{(1 - a)} + \kappa x^2 X = 0,
\]

(33)
\[ K_y \frac{\partial^2 A(y, z)}{\partial y^2} + K_z \frac{\partial^2 A(y, z)}{\partial z^2} + \lambda^2 A(y, z) = 0. \]  
Equation (34), can be expanded in the form:

\[ A_n(y, z) = \sum_{n=0}^{\infty} Y_n(y) \psi_n(z). \]  
Equation (34) can be rewritten as a system of two differential equations as:

\[ \frac{\partial^2 Y_n(y)}{\partial y^2} + \beta^2 Y_n(y) = 0, \]  
and

\[ \frac{\partial^2 \psi_n(z)}{\partial z^2} + \frac{u(z)}{K_z} \left( \lambda^2 - \frac{K_y}{u(z)} \beta^2 \right) \psi_n(z) = 0, \]  
eigenvalues are presented in a more convenient form. The solution for Equation (36) is in the form

\[ Y_\beta(y) = A(\beta) \cos(\beta y). \]  
We recall that \( \gamma, \beta, \lambda \) are the separation constants

\[ \lambda_n^2(x) = \beta_n^2 f_1(x) + \gamma_n^2 f_2(x). \]  
In the case where \( a = 1 \) as regarding classical gaussian equation (29) [45]

\[ \sum_{j=0}^{\infty} \sum_{\text{odd } n=1}^{\infty} \int d y d z = \int_{-y_i}^{h} \int_{y_i}^{h} \]  
According to the above relation, the solution of the initial problem is given in a product form as follows:

\[ c_{\beta}(x, y, z) = \left| \psi_\beta(x) Z_\beta(z) \right| \left| \psi_\beta(y) \right|. \]  
Following this path, the part of the solution of Equation (41) is given by:

\[ \psi_\beta(x, y) = \psi_\beta(y) \exp \left( -\int_0^x \beta^2 f_1(x') dx' \right). \]  
That is,

\[ \psi_\beta(x, z) = \psi_\beta(z) \exp \left( -\int_0^x \gamma^2 f_2(x') dx' \right). \]  
As such, Equation (41) can be recast as:

\[ c_{\beta}(x, y, z) = \int_0^{\infty} B(y) \exp \left( -\int_0^x \gamma^2 f_2(x') dx' \right) A(\beta) \psi_\beta(x) d \beta. \]  
To determine the expressions of the functions \( \psi_\beta(z) \) and \( \psi_\beta(x, y) \), the source term and the initial conditions enable to establish that \( A(0, y) = \delta(y) \) and \( B(0, z) = \delta(z - h_0) \). Then to find the integral related to the eigenvalues \( \beta \). By using the term related to the integral, we derive the following equation:

\[ \psi(x, y) = \int_0^{\infty} A(\beta) \psi_\beta(x, y) d \beta = \int_0^{\infty} A(\beta) \exp \left( -\int_0^x \gamma^2 f_2(x') dx' \right) \cos(\beta y) d \beta. \]  
The application of the initial condition yields:

\[ F(y) = \int_0^{\infty} A(\beta) \chi(\beta, y) d \beta \]  
\[ F(y) \] represents an arbitrary function defined in a semi-interval, with regard to the solution of the auxiliary problem Equation (47). Analogous procedure was found when solving transport diffusion problem [45] by the transformation technique and whose result could be indicated in the form

\[ F(y) = \int_0^{\infty} \chi(\beta, y) \left[ \frac{2}{\pi} \int_0^{\infty} \chi(\beta, y') F(y') dy' \right] d \beta \]  
The above equation is well-founded when \( F(y) \) and \( \frac{dF}{dy} \) are sectionally continuous on each finite interval of the domain. By equating Equations (45) and (46), we obtain the representation of the coefficient \( A(\beta) \)

\[ A(\beta) = \frac{2}{\pi} \int_0^{\infty} \chi(\beta, y) F(y') dy'. \]  
By substituting Equation (47) into Equation (45), the initial solution problem is achieved

\[ \psi(x, y) = \frac{2}{\pi} \int_0^{\infty} \int_0^{\infty} \exp \left[ -\frac{y^2}{2m} \right] \chi(\beta, y) \chi(\beta, y') F(y') dy' d \beta. \]  
\[ \psi(x, y) = \frac{2}{\pi} \int_0^{\infty} \int_0^{\infty} \exp \left[ -\frac{y^2}{2m} \right] \chi(\beta, y') \left( \sin(\beta y') \right) dy' d \beta. \]  
\[ \psi(x, y) = \frac{1}{\pi} \int_0^{\infty} \int_0^{\infty} \exp \left[ -\frac{y^2}{2m} \right] \left( \sin(\beta y') \right) \left( \sin(y'') \right) dy'' d \beta. \]  
Similarly, the following is derived

\[ Z_\beta(z) = B(\gamma) \cos(\gamma z). \]  
\[ \psi(x, z) = \int_0^{\infty} B(\gamma) \psi_\beta(x, z) d \gamma \]  
\[ \psi(x, z) = \int_0^{\infty} B(\gamma) \exp \left( -\int_0^x \gamma^2 f_2(x') dx' \right) \cos(\gamma z) d \gamma. \]  
The application of the initial condition yields

\[ G(z) = \int_0^{\infty} B(\gamma) \chi(\gamma, z) d \gamma \]  
\[ G(z) \] represents an arbitrary function defined in a semi-interval, in terms of the solution of the auxiliary problem. Using the transformation technique, one gets

\[ G(z) = \int_0^{\infty} \chi(\gamma, z) \left[ \frac{2}{\pi} \int_0^{\infty} \chi(\gamma, z') G(z') dz' \right] d \gamma \]
The above equation is well-founded when \( G(z) \) and \( \frac{dG}{dz} \) are sectionally continuous on each finite interval of the domain. By equating Equations (55) and (56), we obtain the representation of the coefficient \( B(y) \)

\[
B(y) = \frac{Q}{\pi} \int_{-\infty}^{\infty} \chi(y, z')G(z')dz'.
\]  
(57)

The substitution of Equation (57) into Equation (54) provides the initial solution problem

\[
\psi(x, z) = \frac{Q}{\pi} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4\pi\alpha} \int_{0}^{z} (z-z')\cos(yz')dz'\right] d\gamma(z')\delta(z-z')
\]

using boundary condition Equation (58)

\[
\psi(x, z) = \frac{Q}{\sqrt{2\pi \alpha}} \exp\left[-\frac{1}{4\pi\alpha} \int_{0}^{z} (z-z')^2 \right] d\gamma(z')
\]

(59)

(60)

(61)

Considering the following underneath relation

\[
\int_{-\infty}^{\infty} \exp\left[-\frac{1}{2\pi\alpha} \int_{0}^{z} dy \right] = \sqrt{2\pi\alpha}
\]  
(62)

the crosswind-integrated solution is given by the upcoming equation:

\[
\psi_{xy}(z) = \frac{Q}{\sqrt{2\pi\alpha\sigma_y}} \exp\left[-\frac{1}{2\pi\alpha\sigma_y} \int_{0}^{z} (z-y)^2 \right] d\gamma(z)
\]

(63)

As noted by Sharan (1998); Hanna and Strimaitis (1990).

In the case where \( 0 < a \leq 1 \), Equation (29) is derived by expecting unidirectional wind. Under moderate to high winds, the flow stemming to longitudinal diffusion Equation (29) is neglected in analogy to advection and accordingly. Equation (29) can be solved using fractional approach solution. Thus, this equation can therefore be transformed using Equation (10) to obtain a known integral form, therefore

\[
u(z) = \frac{C}{\pi} \sum_{n=0}^{\infty} \frac{d^2X_n(x)}{dx^2} \psi_{m,n}(z)
\]

(64)

The analytical solution Equation (64) using boundary conditions Equations (30)-(31) has been obtained by assuming the solution of the form

\[
\psi_{m,n}(z) = \sum_{n=0}^{\infty} X_n(x) \psi_{m,n}(z)
\]

(65)

Where \( X_n(x), n = 0, 1, 2, \ldots \) are the undetermined values of the series. To find these values \( X_n(x) \), we choose solution (65) to satisfy the partial differential equation (64) using the properties from (8) and (9). As result, one gets

\[
\sum_{n=0}^{\infty} \frac{d^2X_n(x)}{dx^2} \psi_{m,n}(z) = \sum_{n=0}^{\infty} \frac{d^2X_n(x)}{dx^2} - u(z)\psi_{m,n}(z)
\]

(66)

Multiplying both sides of the above equation by \( \psi_{m,n} \) (\( n = 0, 1, 2, \ldots \)), and integrating it with respect to \( z \), we obtained the set of first-order Ordinary Differential Equations (ODEs)

\[
\sum_{n=0}^{\infty} \int_{z} \psi_{m,n}(z) \psi_{m,n}(z) d\gamma = \sum_{n=0}^{\infty} \int_{z} \psi_{m,n}(z) \left(-K_z \sigma_y \psi_{m,n}(z) \right) d\gamma + \frac{\delta K_z}{dz} \left( \frac{d\psi_{m,n}(z)}{dz} \right) \right] d\gamma.
\]

(67)

The above equation can be recast in the matrix form

\[
d^zX = \frac{F}{\pi} X,
\]

(68)

for \( z > 0 \) and \( 0 < a \leq 1 \).

Where \( X(x) \) equals a vector, matrix \( F \) is established as \( F = B^{-1}E \), and \( a \) is an arbitrary non-integer value. The components of matrices \( B \) and \( E \) are, respectively,

\[
b_{n,m} = \int_{z} \psi_{m,n}(z) \psi_{m,n}(z) d\gamma
\]

(69)

and

\[
e_{n,m} = \int_{z} \psi_{m,n}(z) \left(-K_z \sigma_y \psi_{m,n}(z) \right) d\gamma + \frac{\delta K_z}{dz} \left( \frac{d\psi_{m,n}(z)}{dz} \right) \right] d\gamma.
\]

(70)

In Equations (68), (69), (70), matrices \( B \) and \( E \) are constant matrices of dimension \( N \times N \). In Equation (68), \( F \) equals \( N \times N \) matrix of the real-valued continuous functions of \( x \) variable. The non-integer dimensions differential equation (68) will have a unique solution [46]

\[
X(x) = E_x \left(-d^x x \right) X_0,
\]

(71)

where \( d_i \) are eigenvalues of matrix \( F \), and \( E_x \) is the Mittag-Leffler function.

\[
E_x \left(-d^x x \right) = \sum_{j=0}^{\infty} \frac{(-d^x x)^j}{\Gamma(j + 1)}
\]

(72)

\( X_0 \) is a known \( N \)-component vector. To determine \( X_0 \), solution (65) is replaced in the source condition (Equation (31))

\[
u(z) \sum_{n=0}^{\infty} X_n(0) \psi_{m,n}(z) = Q \delta(z - H_1).
\]

(73)

Multiplying both sides Equation (73) by eigenfunction \( \psi_{m,n} \) and integrating with respect to \( z \), we get:

\[
\sum_{n=0}^{\infty} \int_{z} \psi_{m,n}(z) \psi_{m,n}(z) d\gamma X_n(0) = Q \psi_{m,n}(H_1)
\]

(74)

or in matrix notation

\[
X(0) = B^{-1} G,
\]

(75)

\( G = Q \psi_{m,n}(H_1) \) equates \( N \times 1 \) matrix column and \( B \) comes from Equation (69). Given a function \( f \) of scalar arguments and a matrix \( F \), the problem of finding a suitable definition for \( f(M) \) goes back to Cayley (1858). For the chosen functional form of \( K_z \) derived in the Equation (11), the matrix \( F \) in Equation (70) could be specified as:
where, $M$ equals square matrix with elements independent of the $x$ variable. Let $M$ be a $N \times N$ matrix with $s$ different eigenvalues $\lambda_1, \ldots, \lambda_s$ and $N_1$ the index of $\lambda_1$, i.e. the smallest integer $q$ so that $(M - \lambda_1 I)^q = 0$, with $I$ denoting the $N \times N$ identity matrix. Therefore, the function $f$ is indicated to be delineated on the A spectrum if the values $f^{(j)}(\lambda_i)$, $j = 0, \ldots, n_i - 1$, $i = 1, \ldots, s$ exist. Thus for functions defined on the spectrum of $M$ the Jordan canonical form could be used to define matrix functions. The $M$ matrix could be altered into the Jordan canonical form as follows [47].

$$M = P J P^{-1}$$

5. Comparison to existing models

To verify the accuracy of the analytical technique developed in the previous section, the solution of Equation (29) represented as Equation (32) behaves well in some special cases. When using particular forms of uniform wind speed. For the rest, we consider the crosswind-integrated concentration. The matrix $B$ equates scalar matrix, i.e. $u$ scalar and $E$ diagonal elements matrix,

$$e_{nn} = -\lambda_n^2 K.$$  \hfill (81)

Therefore, the matrix $F$ in Equation (68) will be a diagonal matrix with diagonal elements

$$d_i = -(K/u) \lambda_n^2.$$ \hfill (82)

In Equation (71), the diagonalisation of matrix $F$ by just integrating diagonal elements yields

$$X_a(s^a) = E_a( -(K/u) \lambda_n^2 s^a) X_a(0).$$ \hfill (83)

### Fig. 1. Convergence of the present model (Equation (64)) and comparison with the exact solution developed by [52].

In the case where in Equation (83) $a = 1$, we end up with the classical exponential solution

$$X_a(x) = \exp \left( -(K/u) \lambda_n^2 x \right) X_a(0).$$ \hfill (84)

Solutions $\psi_n(z)$ $(n = 0, 1, 2, 3, \ldots)$ according to (35) associated to boundary conditions (30) with $\psi_0 = 0$ take the form $\psi_n(z) = b_n \cos(\lambda_n z)$ where $\lambda_n = \frac{n}{h}$, and $b_n$ constant. As a result, starting from the superposition principle, and (31), including the identity below

$$\delta (x - H_j) = \frac{1}{h} \left[ 1 + 2 \sum_{s=1}^{\infty} \cos (\lambda_s H_j) \cos (\lambda_s x) \right].$$ \hfill (85)

the crosswind integrated concentration formula (i.e. $a = 1$) is derived

$$\tilde{c}(x, z) = \frac{Q}{uh} \left[ 1 + 2 \sum_{s=1}^{\infty} \cos (\lambda_s H_j) \cos (\lambda_s x) \exp (-k \lambda_s^2 x) \right].$$ \hfill (86)

finally,

$$\tilde{c}(x, z) = b_0 + \sum_{s=1}^{\infty} b_n \cos(\lambda_n z) E_s(-k \lambda_n^2 x).$$ \hfill (87)

The coefficients $X_a(0)$ in Equation (74) are given by

$$X_a(0) = \frac{Q}{u} \psi_n(H_j).$$ \hfill (88)

In the same vein, Equation (84) leads to the classical Gaussian plume solution (Seinfeld 1986) i.e. an altitudinal source with reflections on two parallel boundaries at points $z = 0$ and $z = h$.

6. Performance of the models

To cross-check the model physical flexibility, this research work laid emphasis on the conventional experimental data from Copenhagen [51]. The experiment happened in Copenhagen in 1978. The tracer was emitted without buoyancy at a height of 115 m and recovered at ground level positions over a maximum of three crosswind arcs of the tracer sampling units.

The site was basically residential with a length of roughness 0.6 m [53]. For practical application, the convergence of solution (13) need to be verified. This is achieved computationally for significant case where $a = 1$. In Fig. 1, we illustrated the evolution of the concentration. It is shown that the concentration becomes almost constant as the
curve increases, and we realised that profile obtained behaved almost as that obtained by (Sharan, 2006). We compared the results achieved by the fractional $\alpha$-GILTT model from the work of (Moreira et al. 2017), against the fractional $\alpha$-Gaussian model from the work of Goulart et al. (2017) and the present $\alpha$-model Figs. 1, 2, 3, 4. In a nutshell, Goulart et al. (2017), focused on a diffusion coefficient that is based on the longitudinal distance, which was considered the average value in this direction. Since the Gaussian model stands for constant coefficients, Moreira and Moret (2017) adopted the diffusion coefficient used throughout the whole PBL given by the formula of Troen and Mahrt, disclosed in the researches of Pleim and Chang (1992), with the mean value for the diffusion coefficient in the vertical direction (height of the PBL). The present model emphasises the modified form of eddy diffusivity as given by (Mooney & Wilson 1993) $K_e(x, z) = f(x)\omega(z)$, where $u(z)$ depicts any form of eddy diffusivity depending on $z$ and $f(x)$ illustrates the correction to $u(z)$ for near source dispersion as dimensionless integrable function of $x$, i.e. a power-law parameterisation of $u(z)$. The micrometeorological conditions used in the initial simulations of this study are those from the experiment conducted at Copenhagen, which one shown in (Table 1), where $u_0$, symbolises the mean wind speed at 10 m, $u_0$ the friction velocity and $L$ the Monin-Obukhov length. These micrometeorological parameters (Table 1) can be obtained from the work of Degrazia et al. (2001) and then collected at 2-3 metres above ground level at positions within a maximum of three crosswind arcs of the tracer sampling units, located 2-6 km from the point of emission. Averaged values of concentrations were measured, three time consecutively about 20 minutes allowing for a total sampling time of 1 hour. Usually, to evaluate the performance of dispersion models, the Environmental Protection Agency (EPA) recommends a well known set of statistical indices (Cox and Tikvart, 1990) defined as follows:

Normalized mean square error (NMSE):

$$NMSE = \frac{(c_p - c_p')^2}{\sigma_p^2}$$

Fractional bias (FB):

$$FB = \frac{(\overline{c}_p - \overline{c}_p')}{0.5(\overline{c}_p + \overline{c}_p')}$$

Correlation coefficient ($R$):

$$R = \frac{(\overline{c}_p - \overline{c}_p')(c_p - c_p')}{\sigma_p \sigma_p'}$$

Fractional variance:

$$FS = \frac{(\sigma_p - \sigma_p')}{0.5(\sigma_p + \sigma_p')}$$

Factor of Two (FA2):

$$FA2 = 0.5 \leq \frac{c_p}{c_p'} \leq 2$$

where $c_p$ and $c_p'$ represented the standard deviations of $c_p$ and $c_p'$, respectively. Where the over bars indicate the average overall measurement terms (N). These parameters focus on the agreement between model predictions and observations (Sharan and Kumar, 2009). A model appears to be perfect for idealised values:

$$NMSE \leq 0.4, -0.3 \leq FB \leq 0.3 \text{ and } COR = FA2 = 1.$$
concentration’s maximum position almost remains invariant. In its arrangement, Figs. 3 and Fig. 4 show the vertical concentration profile for a distance from the point source. This qualitative analysis is used to demonstrate the asymmetry of the turbulent flow with the solution (13). Without the influence of the \( a \) term on the model in Figs. 3 and 4. For the distance closest to the source a few kilometer (1 km), the peak concentration is observed in the region where the source’s height is located, i.e. reinforcing in the present \( a \) model and sharpens when the parameter \( a \) decreases. Like the distance from the source intensifies, notice peak value depletion with a vertical homogenisation propensity. This feature is precisely identified at greater distances than 60 km. At this level, complete concentration homogenisation is observed in the vertical direction, for both \( a = 0.95 \), \( n = 0.90 \) and \( a = 0.85 \), in this direction complete homogenisation has not been ascertained up-to-minute. At all distances simulated, which takes into account continuous wind speed profiles and eddy diffusivity parameters.

Statistical index from mathematical models and results yielded in the Copenhagen dispersion campaign [54] are operated to assess models performance points out in Table 2. In all proposed models, the longitudinal mean wind speed (\( u \)) came from Table 1. In accordance to evolution of concentration depending of distance Fig. 5, present model (87) works much better than \( a \)-GILTT and \( a \)-GM approaches to depict the data of Copenhagen experiment Table 3, as can be experienced from the statistical indices. The present predicted model behaves well than the other models. The correlation factor of \( a \)-GILTT, and \( a \)-GM predicted models equals (0.70, and 0.75 respectively) and present model equals (0.80) in the other hand, the NMSE values as shown in Table 2, indicate for the present and \( a \)-GILTT, \( a \)-GM models 0.03, 0.22 and 0.12. The present model well implemented displays the effect of downwind correction parameter in the vicinity of the source related to eddy diffusivity coefficients.

The \( a \)-present model advantage results from the anomalous diffusion prevailing on turbulence variables with a power-law mean squared distribution. i.e. the local coordinate interchange derivative operator in the fractional transport equation justifies memory effects which appear always in complex systems. At least, with the aim of evaluating the better \( a \) index for the proposed model, we analysed different values of \( a \) varying from \( a = 0.6 \) to \( a = 0.99 \sim 1 \) by steps of 0.05. The best performance occurred when \( a = 0.85 \). As shown in Fig. 2, this \( a \) parameter might gradually not change the maximum value concentration over the time, this reality points out one of the most valuable aspect in studying air contaminants dispersion. The difference between best \( a \) value is confirmed throughout several diffusion coefficients introduced in various cases. This supposes strong correlation among the order and the standard diffusion coefficient for the model to merely characterise observed features. The conventional models (\( a = 1 \)) arise from the molecular diffusion system i.e. Fickian’s law, which supposes Gaussian distribution with linear mean squared displacement for real physical problems, thus asymmetries relevant to turbulent flow embody diffusion coefficients. So far, the fractional exponents characterise anomalous probability distribution with a power-law mean squared fluctuation (87). The anomalous distribution has been proven to be more efficient to perceive particles motion in a turbulent flow [55].

7. Conclusion

The purpose of this work consists in searching the accurate solution of three-dimensional steady-state analytical fractional advection-diffusion equation, for computing air contaminants transport in the PBL. In fact, the introduction of fractional calculus for modeling air pollutants dispersion, nowadays is motivated by the existence of anomalous diffusion due to turbulent flow. We suggest a mere analytical-type fractional differential equation for spatial distribution of air contaminants in PBL. These solutions are achieved by observing a power-law mean

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Table 1. Meteorological conditions during the Copenhagen experiment.

| Exp. | Stability | \( u_0 \) (m s\(^{-1}\)) | \( \alpha \) (m s\(^{-1}\)) | L (m) | \( \sigma_u \) (m s\(^{-1}\)) | h (m) |
|------|-----------|-----------------|----------------|-------|----------------|-------|
| 1    | Very unstable (A) | 2.1 | 0.37 | −46 | 0.83 | 1980 |
| 2    | Slightly unstable (C) | 4.9 | 0.74 | −384 | 1.07 | 1920 |
| 3    | Moderately unstable (B) | 2.4 | 0.39 | −108 | 0.68 | 1120 |
| 4    | Slightly unstable (C) | 2.5 | 0.39 | −173 | 0.47 | 390 |
| 5    | Slightly unstable (C) | 3.1 | 0.46 | −577 | 0.71 | 820 |
| 6    | Slightly unstable (C) | 7.2 | 1.07 | −569 | 1.33 | 1300 |
| 7    | Moderately unstable (B) | 4.1 | 0.65 | −136 | 0.87 | 1850 |
| 8    | Neutral (D) | 4.2 | 0.70 | −72 | 0.72 | 810 |
| 9    | Slightly unstable (C) | 5.1 | 0.75 | −289 | 0.98 | 2090 |

Table 2. Statistical performance indicators of the models for different values of \( a \).

| Dispersion Model | NMSE | PA2 | FB | COR | FS |
|------------------|------|-----|----|-----|----|
| \( a \)-GM       | 0.12 | 0.94 | −0.04 | 0.79 | 0.28 |
| \( a \)-GILTT    | 0.22 | 0.87 | −0.30 | 0.70 | 0.01 |
| Present          | 0.03 | 0.96 | −0.17 | 0.88 | −0.04 |

Table 3. Observed and estimated crosswind-integrated concentrations \( T_0/Q \) (10\(^{-4}\) s m\(^{-1}\)) for Copenhagen experiment.

| Exp. | Distance (m) | Observed | \( a \)-GILTT | \( a \)-Gaussian | Present |
|------|--------------|----------|---------------|-----------------|---------|
| 1    | 1900         | 6.48     | 6.38          | 6.34            | 6.30    |
| 1    | 3700         | 2.31     | 2.47          | 4.95            | 4.10    |
| 2    | 2100         | 5.38     | 4.87          | 4.18            | 4.14    |
| 4    | 2400         | 2.95     | 3.27          | 3.27            | 3.30    |
| 3    | 1900         | 8.20     | 8.70          | 6.51            | 6.45    |
| 5    | 3700         | 6.22     | 5.07          | 5.22            | 5.00    |
| 7    | 3500         | 4.30     | 3.72          | 4.67            | 3.95    |
| 4    | 4000         | 11.70    | 10.75         | 10.70           | 10.60   |
| 5    | 2100         | 6.72     | 4.17          | 5.79            | 5.88    |
| 5    | 4200         | 5.84     | 3.93          | 5.69            | 5.61    |
| 6    | 5100         | 4.97     | 5.00          | 4.48            | 4.10    |
| 6    | 2000         | 3.96     | 2.00          | 2.26            | 2.28    |
| 7    | 4200         | 2.22     | 1.53          | 2.27            | 2.35    |
| 6    | 5900         | 1.83     | 1.17          | 2.06            | 2.13    |
| 7    | 2000         | 6.70     | 2.86          | 4.68            | 5.52    |
| 7    | 4100         | 3.25     | 2.23          | 2.28            | 2.22    |
| 5    | 5300         | 2.23     | 1.95          | 1.73            | 1.70    |
| 7    | 1900         | 4.16     | 4.02          | 3.51            | 4.73    |
| 8    | 3600         | 2.02     | 3.00          | 3.01            | 2.96    |
| 8    | 5300         | 1.52     | 2.94          | 2.29            | 2.18    |
| 7    | 2100         | 4.82     | 2.95          | 2.26            | 2.22    |
| 9    | 4200         | 3.11     | 2.44          | 1.64            | 3.27    |
| 9    | 6000         | 2.59     | 1.95          | 2.00            | 3.15    |
squared fluctuation, in place of a linear one as occurs in the normal diffusion case. The use of realistic wind profiles and vertical eddy diffusivities in distinct kind of atmospheric stratification conditions, leads to an assessment of the performance of the model. Comparison of the $a$-present model against the classical gaussian dispersion model, also as highlighted by the statistical indices, reveals that the diffusion coefficient depends on the distance position from the source point when dealing with the anomalous diffusion. Thus, the initial transformed problem is solved, which gives rise to a more general solution with the introduction of the Mittag-Leffler function, which is fundamentally related to fractional equations.

The fractional problem solution can be reduced to the integer order equation when $a = 1$. In addition, the results obtained from the fractional derivative models could lead to further studies regarding applications of fractional differential systems for modeling the diffusion of airborne contaminants.

**Declarations**

**Author contribution statement**

Tankou Tagne Alain Sylvain: Conceived and designed the analysis; Analyzed and interpreted the data; Contributed analysis tools or data; Wrote the paper.

Ele Abiama Patrice, Ema’a Ema’a’s Jean Marie, Owono Ateba Pierre, Ben-Bolie Germain Hubert: Contributed analysis tools or data.

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