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Prediction of Air Pollution Levels Through Time-Fractional Advection-Diffusion Equation

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Abstract

Traditional models are often not able to capture the (spatial) persistence phenomenon found in air transport so that it is still a challenge predicting the spread of large-scale contamination. In this paper, these long-term effects are accounted for in a one-dimensional time-fractional advection-diffusion equation (Caputo definition) based model. Uniform and non-uniform Dirichlet boundary conditions are applied to test the model. The Eigen function expansion is employed to obtain an analytic solution as it balances mathematical utility and physical understanding. More importantly, it is rigorously shown that the solution is well-posed by utilizing the necessary basic assumptions on the Lipschitz condition with regard to its proofs for the existence, uniqueness, and continuous dependence on the initial input values for the solution. This shows how the fractional calculus could be more precise with regard to the characteristics related to the dispersion of the pollutant in the real world than being confined to the completion of an equation for this task.

Keywords: Grunwald-Letnikov, eigenfunction, fractional time derivatives, numerical simulations, advection-diffusion equation

Mathematics Subject Classifications: 35R11, 35K57, 65M06, 65M12, 76S05.

Introduction

The transport of pollutants between air and water and soil relies on principles of heat transfer and mass transfer. Precise modeling of contaminant transport processes in environmental protection and sustainability are crucial (Baumbach, 2012). The

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atmosphere itself is a source of secondary pollutants due to chemical reactions taking place with direct emissions from traffic and industrial activities and fossil fuel burning. There is established evidence that it poses a threat to human health and natural environments (Kinney, 2018). Indeed, the main limitation in modeling exists with varied environments because pollutants distribute themselves by following non-Fickian or "anomalous" diffusion patterns. The inability to model complicated transport behavior by integer-order advection-diffusion equations leads to a big gap between theoretical prediction and real patterns in the environment (Ndlovu, 2024; Neuman & Tartakovsky, 2009).

The fractional calculus provides the solution to this representation gap. That is, the fractional derivatives, which consist of characteristics of memory-based and long-range dependency, have been suitable in modeling the anomalous transport phenomena arising in nature (Metzler & Klafter, 2000; David et al., 2011). Then, the framework of fractional calculus seems effective in modeling such intricate diffusion patterns in atmospheric and hydrological systems (Tsai & Chen, 2004). One-dimensional time-fractional advection-diffusion equation with variable diffusivity is effective in modeling pollutant dispersion since it handles the complexity of the patterns existing in environmental data (Poudel et al. 2023; Pariyar et al. 2025; Pariyar, S., & Kafle, J. 2024). Solution techniques for the FADE are critical here, as they offer a direct source of robust theoretical understanding, but more importantly, a sound benchmark for simulations. With the imposition of Dirichlet boundary conditions, there are several solution techniques such as the eigenfunction expansion method, useful for predicting the motion of the pollutant, both in a homogeneous or heterogeneous environment, accounting for accurate simulations (Chen & Liang, 2017, Babiarz et al., 2017; Pariyar, S., & Kafle, J. 2022). Far from being neglected is the task of constructing the underlying rigorous theory, whereupon the proof regarding the existence, unicity, and stability aspects under Lipschitz conditions enhances the overall modeling tool itself (Babiarz et al., 2017). Nonetheless, dealing with real-world dispersion problems, especially involving irregular geometries coupled with transient wind velocities, yields closed-form solutions. This, consequently, demands effective numerical solutions. The Grünwald-LeTnikov numerical schemes, developed by Ahmed & Haq, 2024, or the adaptive FE approach by Gao & Liu, 2023, have developed themselves adequately as effective approaches in approximating the FDEs under such complicated geometries. One unmistakable takeaway in such studies is the extreme sensitivity presented by the pollutant distribution, owing to its controlling parameter, the fractional order α, central to the underlying memory aspects Pariyar & Kafle, 2023,2024. Not an entirely remote truth, as it may relate to direct "mathematical truths" surrounding such Fall-Apart Dynamics, is, rather, the profound weighting applied by α, enabling the FADEs, under precise α-manipulation, per se, explaining such long-term memory, persistence, or "reduced mixing" left entirely unaccounted under presentations assuming integer orders. Moving forward along such forays, the paper introduces an analytical-numerical tool support for "air pollution prediction." Hoping, adequately, under such direct analytical insights facilitated by the underlying adjustable numerical tools, such underlying critical work is intended, rather, as it were, its underlying requisites, to offer direct practical understanding, rather, into "air quality analysis, mitigation, or forecasting.

Preliminaries of Fractional Calculus

Definition 1(Ahmed et al. 2024): The Riemann–Liouville fractional integral of order $\alpha > 0$ for a function m(y) is given by

$$ {}_a I^{\alpha}_{y}\, m(y) = \frac{1}{\Gamma(\alpha)} \int_a^y (y-z)^{\alpha-1} m(z)\, dz, \quad y>a, \text{ and} $$

$$ {}_y I^{\alpha}_{a} m(y) = \frac{1}{\Gamma(\alpha)} \int_y^a (y-z)^{\alpha-1} m(z)\, dz, \quad a > y. $$

Definition 2 (Deng et al. 1993): Let ψ(z) be a given function and let $\mu - 1 < \phi < \mu$ with $\mu \in N$. The Riemann–Liouville fractional derivative of order ϕ is defined as

$$ {}^{RL}D^{\phi}\psi(z) = \frac{d^{\mu}}{dz^{\mu}}\left(I^{\mu-\phi}\psi(z)\right) = \frac{1}{\Gamma(\mu-\phi)} \frac{d^{\mu}}{dz^{\mu}} \int_0^z \psi(\eta)(z-\eta)^{\mu-\phi-1}\, d\eta, \quad z>0, $$

where Γ(·) denotes the gamma function and $J^{(\mu)}(\eta)$ represents the μ-th order derivative of ψ.

Definition 3 (Gao. et al., 2023): For $0 < \phi < 1$, the Caputo fractional integral of a function ψ(z) is

$$ I^{\phi}\psi(z) = \frac{1}{\Gamma(\phi)} \int_0^z \psi(\eta)(z-\eta)^{\phi-1}\, d\eta, \quad z > 0. $$

Definition 4 (Pariyar et al. 2024): For a function $J(z)$ and order ∏ satisfying $\mu - 1 < \prod < \mu$, the Caputo fractional derivative is given by

$$ {}^{c}_{0}D^{\phi}_{z}\psi(z) = \frac{1}{\Gamma(\psi-\phi)} \int_0^z \psi^{(\mu)}(\eta)(z-\eta)^{\mu-\phi-1}\, d\eta, \quad \mu-1<\phi<\mu, \quad \text{and for} $$

$$ \phi=\mu, \quad {}^{c}_{0}D^{\mu}_{z}\psi(z) = \frac{d^{\mu}}{dz^{\mu}}\psi(z). $$

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Definition 5 (Pariyar et al. 2023): The single-parameter Mittag–Leffler function $E_\alpha(x)$, where ⟨ is a complex parameter, is defined by

$$E_\alpha(x)=\sum_{k=0}^{\infty}\frac{x^k}{\Gamma(\alpha k+1)}.$$

Analytical Solution of Fractional Advection Diffusion Equation

We consider 1 D, FADE to describe pollutant transport along a spatial domain 0 < x < L, with t > 0 and fractional order 0 < ⟨δ 1 [9]:

$$\frac{\partial^\alpha C(x,t)}{\partial t^\alpha}=D\frac{\partial^2 C(x,t)}{\partial x^2}-u\frac{\partial C(x,t)}{\partial x},$$

where C(x,t) represents the concentration of the pollutant, D is the molecular diffusion coefficient, and u is the advective velocity. The problem is supplemented by the initial and homogeneous Dirichlet boundary conditions:

$$C(x, 0) = f(x),$$

$$C(0, t) = 0, C(L, t) = 0.$$

Since the boundary conditions vanish at x = 0 and x = L, it is natural to represent the solution as a sine-series expansion:

$$C(x,t)=\sum_{n=1}^{\infty}X_n(x)\,T_n(t),\quad X_n(x)=\sin\left(\frac{n\pi x}{L}\right).$$

Substituting into (8) and applying the orthogonality property of sine functions leads to the fractional-order ordinary differential equation:

$\frac{d^\alpha T_n(t)}{dt^\alpha}=-\lambda_n T_n(t),\quad \lambda_n=D\left(\frac{n\pi}{L}\right)^2$. Using the Laplace transform for fractional derivatives, the solution of this equation is obtained as:

$$T_n(t)=A_n E_\alpha(-\lambda_n t^\alpha)$$

where $E_\alpha(\cdot)$ is the Mittag–Leffler function, which generalizes the exponential decay for fractional systems.

The coefficients A_n are determined from the initial condition $C(x, 0) = f(x)$: $A_n = \frac{2}{L}\int_0^L f(x)\ \sin\left(\frac{n\pi x}{L}\right)\ dx$ $\quad An = \frac{2}{L}\int_0^L f(x)\ \sin\left(\frac{n\pi x}{L}\right)\ dx$

can be written as:

$$C(x,t)=\sum_{n=1}^{\infty}\left[\frac{2}{L}\int_0^L f(\xi)\sin\left(\frac{n\pi\xi}{L}\right)d\xi\right]\sin\left(\frac{n\pi x}{L}\right)E_\alpha\left[-D\left(\frac{n\pi}{L}\right)^2 t^\alpha\right]$$

This formulation expresses the pollutant concentration as a superposition of spatial modes, each decaying in time according to the Mittag–Leffler function, which naturally captures the memory effects inherent in fractional-order models. The method provides a compact, closed-form representation that is particularly suited for problems with simple geometries and homogeneous boundary conditions.

Existence and Uniqueness of the Solution

Existence

To demonstrate that the eigen functionssin $\left(\frac{n\pi x}{L}\right)$ form a complete orthonormal basis under homogeneous Dirichlet boundary conditions, consider the integral. For $m\neq n$

$$I_{n,m}=\int_0^L \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx=\frac{L}{2}\left[\left[\frac{\sin\left(\frac{(n-m)\pi x}{L}\right)}{\frac{(n-m)\pi x}{L}}\right|_0^L-\frac{\sin\left(\frac{(n+m)\pi x}{L}\right)}{\frac{(n+m)\pi x}{L}}\Bigg|_0^L\right]$$

Both terms vanish because $\sin(n\pi)=0$ for integ r n,thus $I_{n,m}=0$.

For $n = m$, we have:

$$I_{n,n}=\frac{1}{2}\int_0^L\left[1-\cos\left(\frac{2n\pi x}{L}\right)\right]dx=\frac{L}{2}$$

Hence, the function $\sin\left(\frac{n\pi x}{L}\right)$ are orthogonal. Normalizing them by $\sqrt{\frac{2}{L}}$ ensures their L^2-norm equals 1:

$$\phi_n(x) = \sqrt{\frac{2}{L}}\ \sin\left(\frac{n\pi x}{L}\right)$$

Thus, $\{\phi_n(x)\}$forms an orthonormal basis in $L^2(0, L)$, allowing any function $f(x) \in L^2(0, L)$ to be expanded as:

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$$f(x)=\sum_{n=1}^{\infty}\left[\int_0^L f(x)\phi_n(x)\,dx\right]\phi_n(x).$$

Let $f(x) = C(x,0)$ be the initial condition. The time-dependent coefficients satisfy: $A_n(t)=A_n(0)\,E_\alpha(-\lambda_n t^\alpha)$,

where $E_\alpha(\cdot)$ is the Mittag-Leffler function and $\lambda_n$are the eigenvalues. Since $E_\alpha(z)$ is bounded, the series

$$C(x,t)=\sum_{n=1}^{\infty} A_n(0)E_\alpha(-\lambda_n t^\alpha)\,\phi_n(x)$$

converges uniformly. This ensures that C(x,t) is continuous in t and belongs to $L^2(0,L)$, proving the existence of the solution.

Uniqueness

Let $C_1(x,t)$ and $C_2(x,t)$ be two solutions of the same problem. Define $u(x,t)=C_1(x,t)-C_2(x,t)$. Then u(x,t)satisfies:

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = D\frac{\partial^2 C(x,t)}{\partial x^2} - u\frac{\partial C(x,t)}{\partial x},$$ with homogeneous initial and boundary conditions:

$$u(x,0) = 0, \quad u(0,t) = u(L,t) = 0.$$

Since $u(x,0)=0$ and the problem is linear, it follows that $u(x,t) = 0$ for all x and t.

Thus, $C_1(x,t) = C_2(x,t)$, establishing uniqueness.

1.1.3 Continuous Dependence on Initial Conditions

The solution's dependence on the initial condition f(x) is characterized by the coefficients $A_n(0)$, computed as:

$$A_n(0)=\frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx$$

These coefficients determine the solution C(x,t). Since the Mittag–Leffler function $E_\alpha(-z)$ is bounded, small changes in f(x) result in minor changes in $A_n(0)$ and consequently in C(x,t). We conclude that the problem is well-posed since we have established that the solution C(x,t) depends continuously on the initial condition f(x). Given such a guarantee about the theoretical legitimacy and physical sense of an analytical solution, one naturally turns to the aspect of practical computation in finding approximate solutions and devising numerical schemes applicable for those real-world conditions for which closed-form results are unavailable.

Example

Consider the 1D time-fractional advection-diffusion equation defined over the spatial interval $0 \leq x \leq 1$ and for time $t \geq 0$;

$$\frac{\partial^\alpha C}{\partial t^\alpha} = D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x}, \quad 0<\alpha\leq 1,$$

where the C(x,t) is the constant advection velocity, D is the diffusion coefficient, C(x,t) is the pollutant concentration afractional derivative is taken in Caputo sense. We consider this problem with homogeneous Dirichlet boundary conditions: C(0,t)=0, C(1,t)=0, $\forall t \geq 0$,

We consider this problem with homogeneous Dirichlet boundary conditions:

$$C(x,0)=\sin(\pi x),\ 0\leq x\leq 1.$$

This solution can be represented, via the previously discussed method of eigenfunction expansion, in terms of a Fourier sine series with Mittag-Leffler functions in time:

$$C(x,t)=\sum_{n=1}^{\infty} A_n \sin(n\pi x)\, E_\alpha\left(-D(n\pi)^2 t^\alpha\right),$$

where the coefficients A_n are computed from the initial condition. In this particular case, due to the simple initial function, only the first mode is nonzero with $A_1=1$, yielding the exact closed-form solution:

$$C(x,t)=\sin(\pi x)\ E_\alpha(-D\pi^2 t^\alpha).$$

Consider hydrogen gas as the pollutant with a diffusivity of about $0.00036 m^2/hr$ at 20^oC. in order to show some practical implications of the model. We will evaluate the concentration, taking x=0.4 meters and time t=0.4 hours from the source, assuming $\alpha=0.8$ for capturing the subdiffusive behavior and with a constant wind velocity. Upon numerical evaluation of the above parameters, the pollutant concentration is approximately 0.95314.

The diffusivity parameter D measures the rate at which contaminants disperse across the atmosphere. While the number given is in fact common for a large number of gaseous contaminants, it is important to recognize that realistic diffusivity actually may vary considerably with the pollutant's chemical composition, temperature, humidity,

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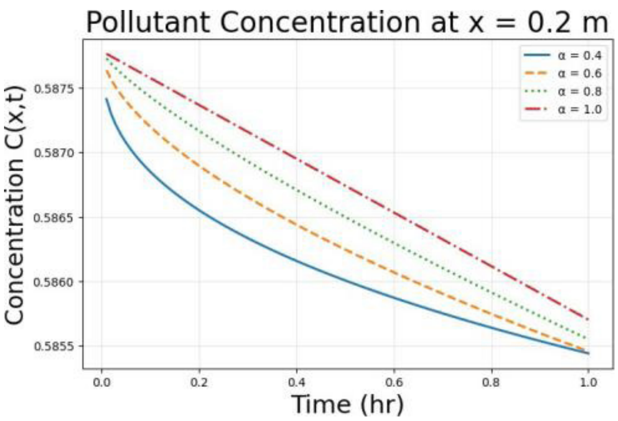
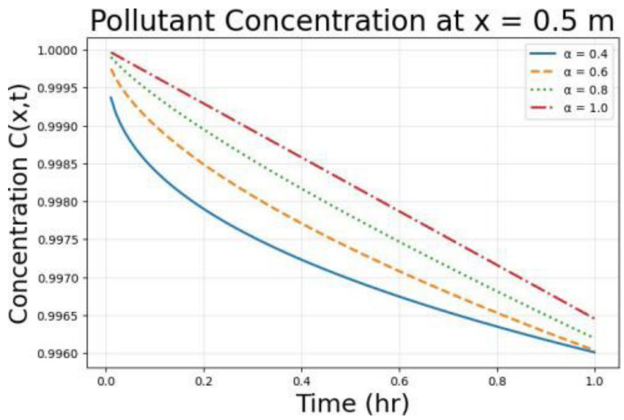
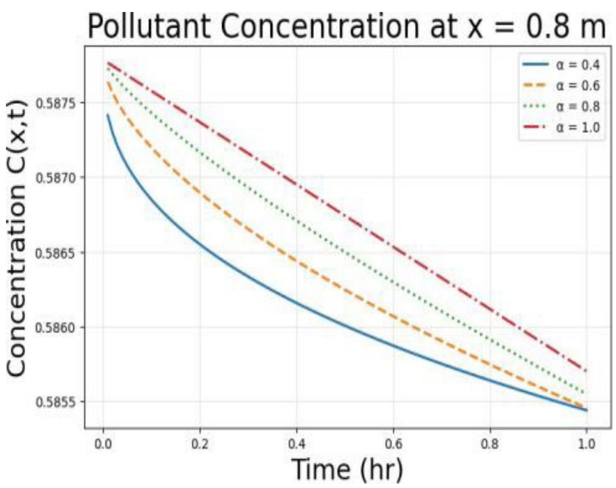
wind conditions, and topography. Fractions introduce the anomalous transport effects commonly encountered in complex air systems and thus offer a more realistic approach to modeling pollutant dispersion.A at x = 0.2m B at x = 0.5m





C at x = 0.8m D at various α and locations



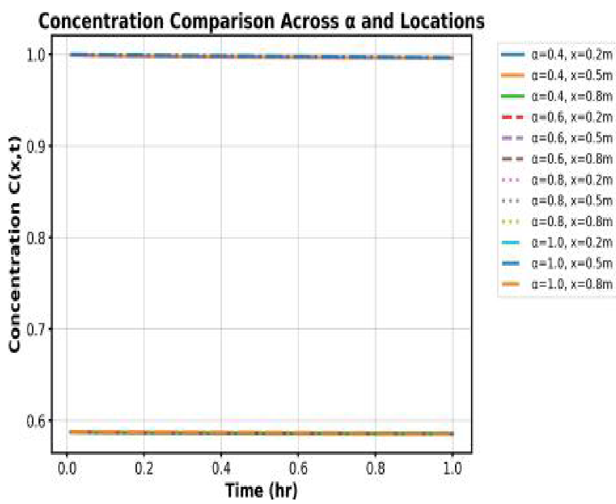


Figure 1: Pollutant concentration over time at location x = 0.2, 0.5, 0.8 m with varying fractional orders α = 0.4, 0.6, 0.8, 1.0.

Our results visually demonstrate how fractional order (α) governs pollutant behavior.

The concentration versus time for x = 0.2 meters from the source is also shown in Figure A. By comparing the curves for α = 0.4, 0.6, 0.8, and 1.0, one can notice that the memory effects are higher and the fall in concentration is slower for smaller α. For example, α = 1 is the case of classical diffusion, and the pollutant gets removed significantly much faster than for α = 0.4, where it remains for a longer period due to fractional dynamics.

This trend continues further away. Plotting the solution 0.5 meters away from the source, Figure B shows generally lower concentrations due to dispersion, but it still clearly displays the large effect of α. Again, delayed decay correlates with smaller values of α indicating that anomalous transport can extend the presence of the pollutant even at half way through the domain.

Figure C 0.8 m, close to boundary, shows this effect is consistent in that even as advection and spreading continue to lower concentrations, lower values of α still tend to slow the decline, showing fractional memory affects transport throughout the entire system.

Figure D combines these observations in a single plot by comparing all locations and all α values. Two relations become immediately evident from the combined view: concentration decreases from the source, and importantly it does so more smoothly as α moves further below 1. This visualization highlights the critical advantage of fractional models: their flexibility in capturing spatially variable persistence.

Key Finding: Fractional derivatives fundamentally alter predicted dispersion. In particular, $\alpha < 1$ introduces memory effects in the model that slow the decay of concentration and therefore prolong the persistence of pollutants at all distances. This result confirms that fractional advection-diffusion equations offer a more realistic and flexible description of anomalous environmental transport than their classical integer-order counterparts.

Conclusion

The method of eigenfunction expansions combined with Mittag-Leffler functions allows us to solve exactly the one-dimensional time-fractional advection-diffusion problem. A unique solution exists and is stable under certain conditions of the problem parameters. The main result indicates that fractional order memory effects ($\alpha < 1$) provide longer residence times and slower degradation rates for pollutants than traditional models predict. The derived result agrees with the anomalous diffusion observed in real environmental systems. Physical accuracy is improved by the validation of the model using hydrogen diffusion parameters. Further research should be directed at the extension of this method to multi-dimensional problems and to problems with space-varying parameters, as well as the determination of practical model parameters. The fractional approach provides a superior mathematical framework, enabling better prediction and control of environmental contamination.

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