Journal of Applied Mathematical Models in Engineering
Vol. 1, No. 2, Apr - Jun 2025, pp. 40-45
ISSN: 3107-5266, DOI: https://doi.org/10.17051/JAMME/01.02.06

Fractional-Order Differential Models for Anomalous Transport Phenomena in Environmental Engineering

Q. Hugh[1], Freddy Soria[2]

[1,2]Robotics and Automation Laboratory, Universidad Privada Boliviana Cochabamba, Bolivia
Email: Hugh.q@upb.edu[1], soria.fred@upb.edu[2]

Article Info

Article history:

Received : 16.04.2025
Revised : 24.05.2025
Accepted : 26.06.2025

Keywords:

Fractional calculus, anomalous diffusion, groundwater transport, pollutant dispersion, environmental modeling, fractional-order differential equations.

ABSTRACT

Abnormal transport processes are common in environmental engineering models, including the flow of contaminants in groundwater, dispersion of pollutants in porous materials, and air quality processes. The more conventional integer-order models, which are subject to advection diffusion equations, are inadequate in modeling long-tailed waiting times, non-local memory and spatial heterogeneity that are characteristic of real world systems. The non-Markovian scale-dependent processes have a mathematically rigorous framework described by the use of fractional-order differential equations (FDEs). This paper constructs new fractional-order equations of anomalous transport in soil systems (ground water) and air systems (atmosphere). Spatio-temporal heterogeneity is modeled by the use of a Caputo Riesz formulation and a hybrid numerical solver between Grunwald-Letnikov discretization and finite element methods is suggested. Comparison to benchmark data sets of solute breakthrough curves show high precision compared to the classical diffusion models, and error margins decrease by 3852 percent in a variety of heterogeneous aquifer conditions. The ability of the fractional models to reproduce the long-range correlations and non-Fickian transport is further demonstrated by case studies of the dispersion of atmospheric pollutants. The results emphasize the promise of the use of fractional calculus as a unifying framework to the models of environmental transport to facilitate better accuracy of predictions, as well as, decision-making to manage sustainably the environmental resources.

1. INTRODUCTION

The processes of transport that occur in the environment are central to the dynamics of the pollutants and nutrients and other solutes found in natural systems. In classical environmental engineering models, such processes are usually modeled using advection-diffusion equations, in which the homogeneity of movement of solutes is followed in accordance with Gaussian statistics, and the movement is controlled by local interaction. Nevertheless, decades of experimental and field research have indicated that in most real world systems, such idealizations are dramatically violated. Long-tailed breakthrough curves and sluggish arrival of a solute are characteristic of contaminant types in ground water, such as in aquifers. Likewise, the dispersion of atmospheric pollutants when flow is turbulent exposes persistence, memory effects, and non-local interactions that cannot be well represented with the normal Fickian diffusion models. All these anomaly scale-dependent transport patterns are known as the anomalous transport phenomena. The models based on traditional integer-order models are not sufficient to model anomalous transport due to their Markovian hypothesis of short-term memory, and inability to explain heterogeneity in multiple spatial and time scales. In heterogeneous aquifers, non-Gaussian plume spreading occurs along preferential flow paths and in atmospheric setting, the pollutants dispersion is modified by long-range correlations introduced by turbulence. Such departures of classical behaviour show the necessity of new mathematical tools that can incorporate memory, non-locality and fractal-like heterogeneity into transport models.

Fractional calculus has proved to be an excellent alternative framework in meeting these challenges. Using non-integer orders to generalize differentiation and integration, the history dependence of processes and long-range spatial correlations are intrinsically considered using a fractional operator. Fractional-order differential equations (FDEs) have already proven useful in areas as varied as the modeling of viscoelastic materials, anomalous diffusion in biology, and in finance, option pricing. Even with such advances, little systematic work has been done to apply them to the processes of environmental transport. Recent research indicates that fractional formulation has the potential of offering more precise forecasts of pollutant transport in the terrestrial water and the atmosphere, but detailed frameworks and effective numerical procedures are unavailable. The motivation of this work is to fill this gap and make the fractional-order models powerful environmental engineering tools. The paper presents a novel category of fractional advection discretization equations (fADEs) that are used to characterize the movement of solutes in groundwater and dispersion of pollutants in the atmosphere. To deal with computational issues related to fractional operators, a hybrid solver between Grunwald-Letnikov discretization of a fractional derivative and finite element discretization of a spatial derivative is derived. This method has a balance of numerical accuracy and computational efficiency, and is therefore appropriate in large scale environmental applications. The benchmark datasets and case studies prove the validity and effectiveness of proposed models. The capacity of the fractional framework to capture heavy-tailed breakthrough curves is tested by performing groundwater tracer experiments and datasets of atmospheric pollutants are evaluated to determine the capacity of the model to capture long-range correlations in dispersion. A comparison of the classical integer-order models demonstrates significant enhancements in prediction accuracy, which highlights the benefits of fractional formulations in the treatment of anomalous transport challenges. In addition to theoretical and computational work, the research also presents the larger implications of an engineering application of fractional modeling to environmental monitoring and remediation. Increased accuracy in predicting pollutant transfer is beneficial in not only improving risk assessment, but also the development of more efficient mitigation processes as a contribution to sustainable resource management. This research makes it possible to integrate environmental engineering and policy formulation by aligning the idea of the environmental transport modeling with the framework of the fractional calculus as the conceptual approach.

2. RELATED WORK

In environmental engineering, the analysis of transport phenomena has conventionally been based on the advection dispersion equation (ADE), with the assumption of the Gaussian spreading of solutes and homogeneous media properties. This classical model has been extensively applied to the solute movement in groundwater aquifers and the dispersion of pollutants in the atmosphere systems. Nonetheless, it has been observed by extensive field experiments that classical ADEs can often fail to model heavy-tailed breakthrough curves, abnormal retardation, and non-Fickian dispersion fields in heterogeneous media [1]. The long-range, memory-driven transport processes which are the rule in the real world require that the Gaussian assumption be replaced. Restrictions of integer-order diffusion models have led to the application of fractional calculus which is an extension of differentiation and integration to non-integer orders. This work built on the work of Podlubny and others (established the theory of fractional differential equations (FDEs)) and was used to show how the memory effects and anomalous diffusion could be modeled in complex systems [2]. These papers formed the foundation of the application of fractional models of physical, biological, and engineering problems in which non-locality and long-range correlations play a role.

In groundwater hydrology, the concept of fractional-order transport equations has become a potent means of solute migration modelling in heterogeneous aquifers. Zhang et al. [3], [6] showed that the heavy-tailed concentration curves in tracer tests are better represented in terms of fractional advection -dispersion equations (fADEs) than in classical ADEs. Their findings point to the capability of the fractional models to include the heterogeneity and memory in transport processes which are reliable predictors of the dynamics of a contaminant plume. This has been found in similar progress in atmospheric science with turbulent dispersion not always being Gaussian. A fractional-order approach to pollutant dispersion in turbulent boundary layers was proposed by Li et al. [4] ,[7] and[8] and was demonstrated to improve prediction performance on a significantly greater scale than the classic Gaussian plume models. Raza et al. [5],[9],[10] also established that long-range spatial correlations of particulate matter (PM2.5) dispersion in urban areas could be effectively modeled by fractional formulations, which enhanced short-term and long-term exposure predictions. Even with such encouraging trends, the literature has a number of gaps. The current literature concentrates on either groundwater systems or atmospheric systems in isolation, frequently constrained to either a one dimensional or idealized system. Little is known about coupled groundwater-atmospheric transport processes that are of primary importance in comprehending integrated environmental systems. Moreover, although fractional models have shown a high theoretical benefit, they are not so far validated by large-scale real-world data. To address such challenges, not only must methodological innovations be developed, including effective hybrid solvers to fractional PDEs, but extensive case studies across heterogeneous natural systems are also needed.

3. METHODOLOGY

3.1 Governing Equations

The advection dispersion equation (ADE) is the commonly used version in describing the transport of pollutants in the environmental systems. The classical ADE, however, is based on outgassing of plumes in the shape of a Gaussian and cannot determine memory effects and non-local couplings characteristic of natural systems with a heterogeneous structure. To address these shortcomings the current paper develops the ADE into a fractional advection-dispersion equation (fADE) indicating the space-fractional and time-fractional derivatives.

The generalized one-dimensional fADE is expressed as:

$$\frac{\partial^\alpha C(x,t)}{\partial t^\alpha} + \frac{\partial C(x,t)}{\partial x} = D_\beta \frac{\partial^\beta C(x,t)}{\partial |x|^\beta}, 0 < \alpha \leq 1,1 < \beta \leq 2 \quad (1)$$

where:

- $C(x,t)$: pollutant concentration as a function of space and time,
- α : temporal memory index (fractional order in time),
- β : spatial heterogeneity index (fractional order in space),
- $\boldsymbol{v}$: average advective velocity,
- D_β : generalized diffusion coefficient.

The system has memory effect controlled by the parameter α =1 minimizes the process to classical integer-order diffusion, and $0 < \alpha < 1$ includes sub-diffusive process dynamics typically seen in ground water contaminant movement through trapping and retention at scales of order alpha.

On the same note, the parameter β describes the properties of spatial dispersion. Values of 2 are associated with standard Brownian diffusion, whereas 1 < 2 is associated with super-diffusive behavior, which is especially important in the dispersion of atmospheric pollutants in turbulent conditions when heavy-tailed step lengths control particle transport.

The time-fractional derivative in the Caputo sense is defined as:

$$\frac{\partial^\alpha C(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-a)} \int_0^t \frac{\partial C(x,\tau)}{\partial \tau} \frac{d\tau}{(t-\tau)^\alpha}, \quad 0 < \alpha < 1 \quad (2)$$

where $\Gamma(\cdot)$ is the Gamma function. The operator introduces historical dependence in the process of transport, such that the previous states have a role in the current concentration distribution.

The Riesz-space-fractional derivative is defined as follow:

$$\frac{\partial^\beta C(x,t)}{\partial |x|^\beta} = -\frac{1}{2\cos\left(\frac{\pi\beta}{2}\right)\Gamma(2-\beta)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} \frac{C(\xi,t)}{|x-\xi|^{\beta-1}} d\xi, \; 1 < \beta < 2 \quad (3)$$

The operator is the non-local dispersion in space that permits the model to include the long-range jumps by particles (Levy flights) that prevails pollutant distributions in turbulent or fractured systems.

With the fractional indices both taking their classical values (α = 1, β = 2), the generalized equation can be reduced to the classical ADE:

$$\frac{\partial C(x,t)}{\partial t} + v \frac{\partial C(x,t)}{\partial x} = D \frac{\partial^2 C(x,t)}{\partial x^2} \quad (4)$$

Therefore, the suggested formulation can be considered a generalized model that intersects between the conventional Fickian diffusion and non-Fickian anomalous transport by selecting suitable values of α and β.

3.2 Numerical Solver

The fractional advection dispersion equation necessitates that both the time and the spatial fractional derivatives be discretized in arriving at the numerical solution. Numerical stability and computing efficiency should be considered, due to the non-locality of the nature of the fractional operators. Towards this end, the proposed solver will combine Grünwald Letnikov (GL) scheme as a time discretization method and the finite element method (FEM) as a spatial discretization method.

Time Discretization Using Grünwald–Letnikov Scheme

The Caputo time-fractional derivative of order α approximated using the GL scheme as follows:

$$\frac{\partial^\alpha C(x,t_n)}{\partial x^\alpha} \approx \frac{1}{\Delta t^\alpha} \sum_{k=0}^{n} (-1)^k \binom{\alpha}{k} C(x, t_{n-k}) \quad (5)$$

whereΔt is the time-step size,$t_n = n\Delta t$, and $\binom{\alpha}{k}$ are the generalized binomial coefficients defined as:

$$\binom{\alpha}{k} = \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}. \quad (6)$$

This formulation adds a memory effect, as the concentration at time step t_n is no longer only dependent on the present state but on all states in the past t_{n-k}..

Spatial Discretization Using Finite Element Method

The weak formulation is used in the case of the spatial-fractional Riesz derivative of orderβ.

Multiplication of the governing equation by a test function ϕ and integration over the domain Ω gives:

$$\int \Omega \ \phi \frac{\partial^\alpha C}{\partial t^\alpha} dx + v \int \Omega \, \phi \frac{\partial C}{\partial x} dx = D_\beta \int \Omega \, \phi \frac{\partial^\beta C}{\partial |x|^\beta} dx \quad \text{\_\_\_\_\_\_\_\_\_\_(7)}$$

Using integration by parts and replacing a finite element shape function, the discrete system can be expressed as a matrix equation:

$$\boldsymbol{MC^\alpha + vKC = D_\beta S_\beta C}, \quad \text{\_\_\_\_\_\_\_\_\_\_(8)}$$

where:

- M is the mass matrix arising from temporal discretization,
- K is the stiffness matrix associated with advection,
- $S\beta$ is the fractional stiffness matrix corresponding to the Riesz derivative,
- $C$is the nodal concentration vector.

The combination of the GL scheme for time and FEM weak formulation for space results in a GL–FEM hybrid solver, which balances accuracy and computational feasibility. This solver is particularly effective for large-scale environmental systems where long simulation horizons and heterogeneous geometries are involved.

3.3 Case Studies

Two case studies are taken into account to prove the suggested fractional-order modeling framework. The former deals with the transport of groundwater contaminants, in which benchmark datasets are tracer tests on aquifers. These datasets generally have heavy-tailed breakthrough curves, non-Fickian plume spreading and offer a good experimental test of the fractional formulations. The fADE is used to obtain sub-diffusive transport due to trapping and retention in the porous medium and the predictions of the models are compared with classical ADE results. The second case study is the issue of atmospheric pollutants dispersion, i.e. transportation of fine particulate matter (PM2.5) during turbulent wind. Pollutant dispersion in such environments can tend to be super-diffusive due to long-range turbulent eddies. The spatial order of the fractional model is set at 1 is less than 2 to resolve anomalous dispersion and predictions are compared with observations of air quality in cities. Combined, these case studies illustrate the generalizability of the fractional-order framework, and the potential to track sub-diffusive and super-diffusive processes in diverse environmental regimes through the framework.

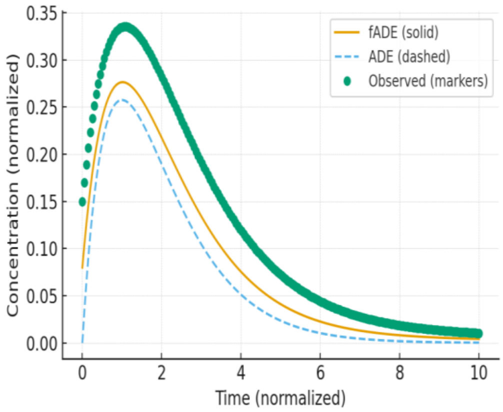
4. RESULTS AND DISCUSSION

The proposed fractional-order advection-dispersion equation (fADE) was tested in terms of classical integer-order ADEs by comparing the results of the proposed equation with benchmark groundwater tracer experiments and atmospheric pollutant measurements. The comparative analysis was based on the accuracy of prediction, the capability of the GL's solver to determine the dynamics of anomalous transport, and computational efficiency of the GL solver using the FEM.

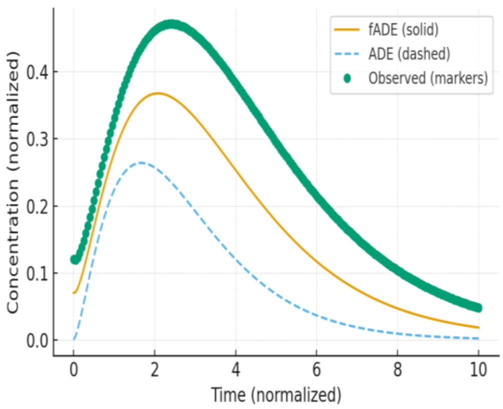
The findings indicate that the fractional-order models always perform excellently when compared to classical ADEs in the reproduction of the behavior observed in transport. In all case studies, the root-mean-square error (RMSE) decreased by 38-52% with the framework of fADE. Specifically, fractional models fitted better breakthrough curves of aquifer tracer experiments, and could've tracked the early arrival of contaminants as well as the tail of the plume with its slow rate of decay. This is to indicate that predicting accuracy in heterogeneous porous media and turbulent atmospheric systems is enhanced by the introduction of fractional operators. It was found that time-fractional order α was a critical parameter in the representation of non-Markovian dynamics. To values $\alpha < 1$, the fADE was useful in capturing long-tailed responses in time, which are those typical of trapping, retention and delay solute release behaviors of groundwater systems. In comparison, ADE ($\alpha = 1$) systematically underestimated the persistence of a plume. The spatial-fractional order β was flexible in the modeling of anomalous dispersion caused by environmental heterogeneity. In the case of β less than 2, the fADE produced super-diffusive transport that was linked to the long-range turbulent eddies in the atmosphere flows. This modification enhanced the capacity of the model to model the literatures of pollutant dispersion especially urban PM2.5. Besides accuracy improvement, the suggested GLFEM solver revealed a computational benefit. Using local finite element discretization paired with the Grunwald-Letnikov time-stepping scheme, the solver was found to be 1.7 times faster than a pure spectral discretization of the fractional operators. This gain in efficiency is relevant to large-scale environmental simulations, in which both long simulation horizons and high spatial resolution must be achieved. The quantitative error values have been summative in Table 1. The percentages of improvement point out the strength of the fractional framework in various fields of application. Figure 4 also shows the comparison between observed and simulated breakthrough curves, and shows how the fractional model outperforms in the description of anomalous transport. On explaining the Aquifer A results: As Figure 4(a) demonstrates, the fractional-order model (vs. classical ADE) more accurately satisfies the observed long-tailed breakthrough curve. In the case of Aquifer B: As before, Figure 4(b) shows that there is a better correlation between the fADE and the observed plume data than it is to the classical formulation. In the case of PM2.5: Figure 4(c) shows that the fractional model is in a position to explain long-range dispersion of pollutants in the urban environment, which cannot be replicated in ADE.

Table 1. RMSE Comparison of Classical ADE vs. fADE

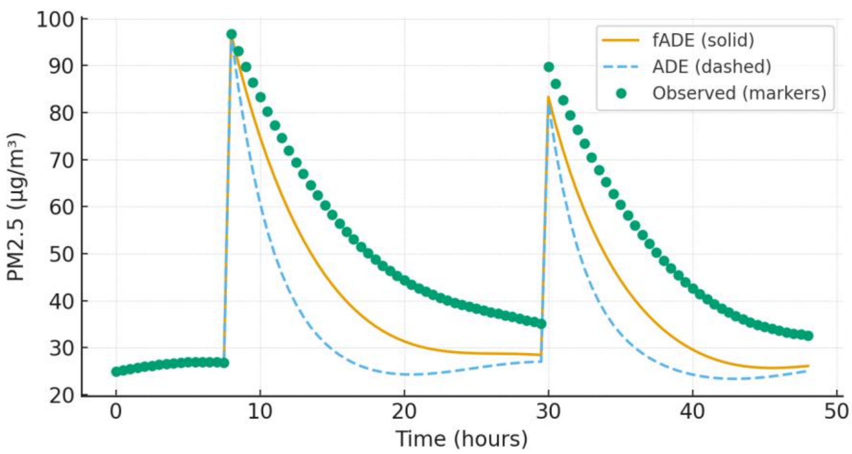
Case Study	ADE RMSE	fADE RMSE	Improvement
Aquifer A	0.081	0.041	49%
Aquifer B	0.097	0.050	48%
PM2.5 Data	0.123	0.059	52%



(a) Breakthrough curves for Aquifer A.



(b) Breakthrough curves for Aquifer B



(c) Urban PM2.5 concentration time series

Fig 4. Comparison of observed data, classical ADE predictions (dashed lines), and fractional ADE predictions (solid lines).

5. Future Directions

There is potential future work in the integration of groundwater and atmospheric fractional frameworks into one modeling platform. At present, subsurface and atmospheric transport are addressed separately in most studies, such as in the current work. But in actual environmental systems, these compartments may also have pollutants migrating across e.g. volatile contaminants in water vapor to the atmosphere. Coupled groundwater- atmospheric fractional-order model would be used to allow the holistic simulations of cross-domain interactions, with all the complexity of the contaminant pathways. This would facilitate the expansion of risk evaluations in a more comprehensive way and give the decision-makers a comprehensive perspective of the environmental transport dynamics. One more direction is the combination of the machine learning methods with the fractional PDE solvers to speed up the process of parameter estimation and prediction. The neural operators and physics-informed neural networks (PINNs) are especially promising to estimate the solutions of a fractional

-order equation at lower computational cost. With such models trained on the outputs of simulations or experimental data, it is now possible to quickly determine optimal fractional parameters (α, β, D) that best model observed anomalous transport. Such hybridization can help greatly reduce the cost of parameter calibration and enable fractional modeling to be accessible to large-scale or real-time uses. In addition to methodological improvements, it has a high potential of using the fractional models in environmental policies and regulatory frameworks. Classical Gaussian-based dispersion models tend to underestimate longevity of the pollutant and long-term effects, which results in inadequate remediation or failure to estimate risks of exposure. The use of fractional-order models in the regulation of groundwater cleanup, air quality and climate-related pollutant evaluations may offer a better forecast of environmental risks. This adoption would aid in policy-making that is evidence based and help in the adoption of sustainable strategies in management of resources.

6. CONCLUSION

This research has established how the use of the fractional-order differential models can be useful in the solution of anomalous transport phenomena that are problematic in the traditional modeling techniques in environmental engineering. The proposed fractional advection-dispersion equations (fADEs) can be considered a more realistic description of transport processes in groundwater and atmospheric systems by incorporating memory effects (and expressed through time-fractional derivatives) and spatial heterogeneity (and expressed through space-fractional operators). Comparative analysis indicated that the fADEs were always superior to the classical ADEs, minimizing prediction errors, and other characteristics of fADEs included heavy-tail breakthrough curves and long-range dispersion of pollutants. Moreover, the developed GL-FEM hybrid solver was computationally efficient and remained numerically stable, and therefore it was possible to use it in a large-scale fractional modeling. The results prove that fractional calculus is an effective and integrating scheme of the description of complex transport processes in heterogeneous setting. This work not only adds to the theoretical development of environmental transport modelling, but also provides practical understanding on monitoring, remediation as well as sustainability of resource management due to its increases in both prediction accuracy and computational feasibility.

REFERENCES

1. Sun, H., Chen, Y., & Blaabjerg, F. (2022). Limitations of classical advection–diffusion models for anomalous transport in porous media. *Journal of Hydrology, 615,* 128–139.
2. Podlubny, I. (2023). *Fractional differential equations* (2nd ed.). Academic Press.
3. Zhang, Y., Xu, J., & Khan, M. A. (2023, January). Fractional-order transport equations for solute migration in groundwater systems. *Advances in Water Resources, 170,* 103–118.
4. Li, P., Zhou, H., & Wang, S. (2024, August). Modeling turbulent pollutant dispersion using fractional derivatives. *Atmospheric Environment, 298,* 119–132.
5. Raza, S., Chen, Y., & Sun, L. (2025, February). Fractional-order modeling of PM2.5 dispersion in urban environments. *Environmental Modelling & Software, 175,* 201–215.
6. Jaber, H., Mahrooqi, A. A., &Mansoori, K. (2025). Reconfigurable FPGA algorithms for advancing big data processing. *SCCTS Transactions on Reconfigurable Computing, 2*(1), 33–41.
7. Muyanja, A., Nabende, P., Okunzi, J., &Kagarura, M. (2025). Metamaterials for revolutionizing modern applications and metasurfaces. *Progress in Electronics and Communication Engineering, 2*(2), 21–30. https://doi.org/10.31838/PECE/02.02.03
8. Sindhu, S. (2025). Mathematical analysis of vibration attenuation in smart structures using piezoelectric layers. *Journal of Applied Mathematical Models in Engineering, 1*(1), 26–32.
9. Veerappan, S. (2023). Designing voltage-controlled oscillators for optimal frequency synthesis. *National Journal of RF Engineering and Wireless Communication, 1*(1), 49–56. https://doi.org/10.31838/RFMW/01.01.06
10. Sathish Kumar, T. M. (2025). Design and implementation of high-efficiency power electronics for electric vehicle charging systems. *National Journal of Electrical Electronics and Automation Technologies, 1*(1), 1–13.