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Time-Fractional Differential Operator Modeling of Contaminant Transport with Adsorption and Decay

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Abstract

In this work, the advection-dispersion model (ADM) is time-fractionalized by the exploitation of Atangana-Baleanu (AB) differential operator to describe contaminant transport in a geological environment. Dispersion, adsorption, and decay, which are known as the foremost transport mechanisms, are considered. The exact solutions of the suggested Atangana-Baleanu advection-dispersion models (AB-ADMs) are acquired using Fourier sine transform and Laplace transform. The classical ADMs are demonstrated to be the special limiting cases of the suggested models. The high consistency among the suggested models and experimental data denotes that the AB-ADMs characterize contaminant transport more effectively. Additionally, the corresponding numerical and graphical results are explored to demonstrate the necessity, effectiveness, and suitability of the suggested models.

Keywords: Atangana-Baleanu differential operator; advection-dispersion; contaminant transport; adsorption; first-order decay

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1. Introduction

Efforts to inhibit or even prevent the migration of a contaminant through the geological system have always been the focus of safe treatment and disposal of contaminants. Researchers with diverse backgrounds in hydrology, geology, soil science, engineering, physics, chemistry, statistics, and mathematics have undertaken a broad range of theoretical, numerical, laboratory, and field investigations [1]. Many issues focusing on migration of contaminants have been addressed, from a variety of perspectives. It is found that, due to the complex contaminant migration mechanism, the diversity of surrounding rock selection, the heterogeneity of geological body, the complexity and variability of groundwater flow field, and so on, multiple mechanisms, including convection, dispersion, adsorption, and decay, need to be considered in the establishment of contaminant diffusion models [2], which means the analytical solutions of solute transport models considering multiple mechanisms are expressed in more complicated forms [3]. Then, it is a key point to establish

the contaminant transport models to portray the process of contaminant transport more accurately. At the same time, the experimental research on the migration of a contaminant is in progress; Ajayi et al. [4] and Krsti et al. [5] investigated the vertical distribution of Cesium in soil. Pang and Casey et al. [6,7] discussed the solute transport with sorption and degradation, while Chen et al. [8,9] studied the migration of radionuclides in granite. A great deal of experimental studies indicated that the contaminant migration in porous media reveals a long-tail phenomenon [10–12], which cannot be captured via the traditional contaminant transport models. As a result, the improvement of contaminant transport models is necessary.

On the other hand, the fractional derivative [13] emerged as an idea of generalization of the classical derivative definition, and it has become a key tool in engineering modeling [14–17]. The non-locality property of the fractional derivative makes problems fractionalized so that they are more functional and precise in relation to the classical cases, and it turned out to yield obvious advantages in describing the long-tail phenomenon and time-dependence characteristics [18,19]. Convincing evidence in much literature has shown that the typical deviations from classical ADM (power-law decay in breakthrough curves) can be amended by introducing fractional operators. The well-known fractional derivative definition, the Caputo derivative [20], has wide applications in many fields, such as non-Darcian flow [21], contaminant transport [22], and the viscoelastic model and diffusion [23,24], due to the fact that the Caputo derivative is not necessary to define fractional-order initial conditions when solving the differential equations. Unlike the Caputo derivative definition based on power-law kernel with singularity; in the last decade, some new non-singular differential operators have been proposed. Caputo and Fabrizio [25] proposed a differential operator with an exponential kernel. The Caputo–Fabrizio differential operator has been employed in a number of areas, for instance, fluid flow [26,27], the virus model [28,29], and the human liver model [30]. Recently, Atangana and Baleanu [31] put forward a new non-local and non-singular fractional operator employing the Mittag–Leffler function as its kernel, which aims to describe the full memory effect in systems since the Mittag–Leffler function features exponential and power-law decay at short and long time scales, respectively. It is widely used to describe real-world problems [32–36].

The diffusion model is the basic and classical model for describing solute transport. In order to describe a realistic transport phenomenon in a geological system, the solute transport models in porous media usually consider diffusion, advection, and other reactions. Apart from the diffusion model forms, the continuous-time random walk model [37], which is often discussed in physics, the multirate mass transfer model [38], fractional mobile–immobile models [39], and stochastic streamtube approaches [40] are frequently used in the literature. Considering first-order decay, adsorption, and advection to the diffusion model of the contaminant, which is also called the advection–dispersion model (ADM), the objective of this work is expected to provide generalized models of contaminant migration in geological environment associated with the Atangana–Baleanu (AB) differential operator to develop and analytically solve AB-fractional advection–dispersion equations with adsorption and decay and to validate them against benchmark experimental datasets. The relative experimental data are used to fit the obtained analytical solution, and the corresponding numerical pictures give a clear description of the results shown in this work. The commonly used solutions of ADM are shown to be the special cases of the proposed model.

The rest of this work is organized as follows. In Section 2, the advection–dispersion model with Atangana–Baleanu differential operator (AB-ADM) is proposed. In Section 3 and Section 4, the AB-ADMs with linear adsorption and first-order decay for describing contaminant transport are introduced, respectively, and the accurate analytical solutions are

obtained. Moreover, the related experimental data are displayed to acquire the fitting results with the analytical solutions. Furthermore, the relevant numerical and graphical results are explored to demonstrate the necessity, effectiveness, and suitability of the suggested models. In Section 5, the limitations and further extensions of AB-ADM are discussed. In Section 6, the conclusions are drawn. In Appendix A, the basic integral transforms and formula used in this work are given.

2. Advection-Dispersion Models with Atangana–Baleanu Differential Operator

In this section, we build the advection–dispersion model by using the AB differential operator to depict the contaminant transport in a geological environment.

2.1. Advection-Dispersion Model

The basic formulation of flow and transport in porous media has been intensively studied by researchers from the theoretical and simulation levels. The classical one-dimensional advection–dispersion model to describe contaminant transport is represented as [41,42]

$$\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2} - u \frac{\partial C(x, t)}{\partial x} + R_s(x, t), \quad (1)$$

where $C(x, t)$ is the concentration function, D is the diffusion coefficient, u is convective velocity, and $R_s(x, t)$ represents arbitrary sinks or sources of solute, such as adsorption, first-order decay, and production.

2.2. Atangana–Baleanu Differential Operator

The well-known Caputo derivative [20] can be interpreted as the convolution of the first derivative of function $f(t)$ and the power-law function, i.e., ${}_0^C D_t^\alpha [f(t)] = \int_0^t f'(u) M_C(t-u) du$, where $M_C(t) = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}$, which is also known as the memory kernel. Changing the memory kernel to the exponential function, i.e., $M_{CF}(t) = \frac{1}{1-\alpha} \exp\left[\frac{-\alpha t}{1-\alpha}\right]$, it denotes the Caputo–Fabrizio differential operator [25], when the memory kernel is $M_{AB}(t) = \frac{1}{1-\alpha} E_\alpha\left[-\frac{\alpha t^\alpha}{1-\alpha}\right]$, it represents the Atangana–Baleanu differential operator [31] defined by

$${}_0^{AB} D_t^\alpha [f(t)] = \frac{1}{1-\alpha} \int_0^t f'(u) E_\alpha\left[-\alpha \frac{(t-u)^\alpha}{1-\alpha}\right] du, \quad (2)$$

Here, $E_{\alpha, \beta}(x) = \sum_{j=0}^{\infty} \frac{x^j}{\Gamma(\alpha j + \beta)}$ is called Mittag–Leffler function [43]. In particular, $E_{\alpha, 1}(x) = E_\alpha(x)$, $E_1(x) = e^x$.

These newly defined differential operators have been applied to model radionuclide anomalous transport [33] and non-Darcian flow [27], from which we conclude that the AB differential operators could better fit with the relative long-time memory effect. Moreover, the essential integral transformations used can be referred to in Appendix A.

2.3. Advection–Dispersion Models with AB Differential Operator

Integrating the AB differential operator into Equation (1), the one-dimensional AB-ADM for contaminant transport can be derived as

$${}_0^{AB} D_t^\alpha [C(x, t)] = D_\alpha \frac{\partial^2 C(x, t)}{\partial x^2} - u \frac{\partial C(x, t)}{\partial x} + R_s(x, t). \quad (3)$$

Considering the following conditions in virtue of engineering practices,

$$\begin{aligned}
C(x, 0) &= 0, \\
C(0, t) &= C_0[1 - \varepsilon(t - t_0)], \\
C(\infty, t) &= 0, \\
\frac{\partial C(\infty, t)}{\partial x} &= 0,
\end{aligned} \tag{4}$$

D_α is the generalized diffusion coefficient, $\varepsilon(t)$ is the unit step function [44], C_0 is the injected concentration, t_0 is the duration of injection.

3. The AB-ADM with Linear Adsorption

If it is supposed that contaminant transport with linear adsorption $S(x, t) = aC(x, t)$, then the sinks or source term can be referred to as

$$R_s(x, t) = \frac{n-1}{n} {}_0^{AB}D_t^\alpha [S(x, t)] = \left(\frac{n-1}{n} a \right) {}_0^{AB}D_t^\alpha [C(x, t)], \tag{5}$$

where $S(x, t)$ is the adsorbed concentration in a solid phase, and n refers to the porosity of the porous medium.

Combining Equation (5) with Equation (3) leads to the following AB-ADM with linear adsorption:

$$R \left\{ {}_0^{AB}D_t^\alpha [C(x, t)] \right\} = D_\alpha \frac{\partial^2 C(x, t)}{\partial x^2} - u \frac{\partial C(x, t)}{\partial x}, \tag{6}$$

$R = 1 + \frac{1-n}{n}a$ is the retardation factor (when $R = 1$, no adsorption phenomena are considered).

Introducing the new function $C(x, t) = K(x, t) \exp(\frac{ux}{2D_\alpha})$, one can obtain

$$R \left\{ {}_0^{AB}D_t^\alpha [K(x, t)] \right\} = D_\alpha \frac{\partial^2 K(x, t)}{\partial x^2} - \frac{u^2}{4D_\alpha} K(x, t). \tag{7}$$

When F.S.T. and L.T. are applied to Equation (7), conditions Equation (4), and considering Equations (A2), (A5), and (A7), we derive

$$\frac{R s^\alpha}{(1-\alpha)s^\alpha + \alpha} \tilde{K}(\xi, s) = D_\alpha \left[-\xi^2 \tilde{K}(\xi, s) + \sqrt{\frac{2}{\pi}} \xi \tilde{f}(s) \right] - \frac{u^2}{4D_\alpha} \tilde{K}(\xi, s), \tag{8}$$

that is,

$$\tilde{K}(\xi, s) = \frac{\sqrt{\frac{2}{\pi}} D_\alpha \xi \tilde{f}(s)}{\frac{R s^\alpha}{(1-\alpha)s^\alpha + \alpha} + D_\alpha \xi^2 + \frac{u^2}{4D_\alpha}}, \tag{9}$$

where $\tilde{f}(s) = C_0 \frac{1}{s} [1 - \exp(-st_0)]$.

Employing the I.F.S.T. and inverse L.T. to Equation (9), and utilizing Equations (A3) and (A4), we infer that

$$K(x, t) = \begin{cases} K_1(x, t) & 0 < t \leq t_0 \\ K_1(x, t) - K_1(x, t - t_0) & t_0 < t < +\infty \end{cases}, \tag{10}$$

where $K_1(x, t) = C_0 \exp\left(-\frac{ux}{2D_\alpha}\right) - \frac{2}{\pi} C_0 \int_0^\infty \frac{\xi B}{\xi^2 + \frac{u^2}{4D_\alpha^2}} E_\alpha(-A t^\alpha) \sin(\xi x) d\xi$, with

$$A = \frac{\alpha(D_\alpha \xi^2 + \frac{u^2}{4D_\alpha})}{R + (1-\alpha)(D_\alpha \xi^2 + \frac{u^2}{4D_\alpha})}, \text{ and } B = \frac{1}{R + (1-\alpha)(D_\alpha \xi^2 + \frac{u^2}{4D_\alpha})}.$$

Consequently, the analytical solution of Equation (6) is

$$C(x, t) = \begin{cases} C_1(x, t) & 0 < t \leq t_0 \\ C_1(x, t) - C_1(x, t - t_0) & t_0 < t < +\infty \end{cases}, \quad (11)$$

where $C_1(x, t) = C_0 - \frac{2}{\pi} C_0 \exp\left(\frac{ux}{2D_\alpha}\right) \int_0^\infty \frac{\xi B}{\xi^2 + \frac{u^2}{4D_\alpha^2}} E_\alpha(-At^\alpha) \sin(\xi x) d\xi$.

Figure 1 shows the concentration distributions of AB-ADM with linear adsorption in Equation (11) for different fractional index α .

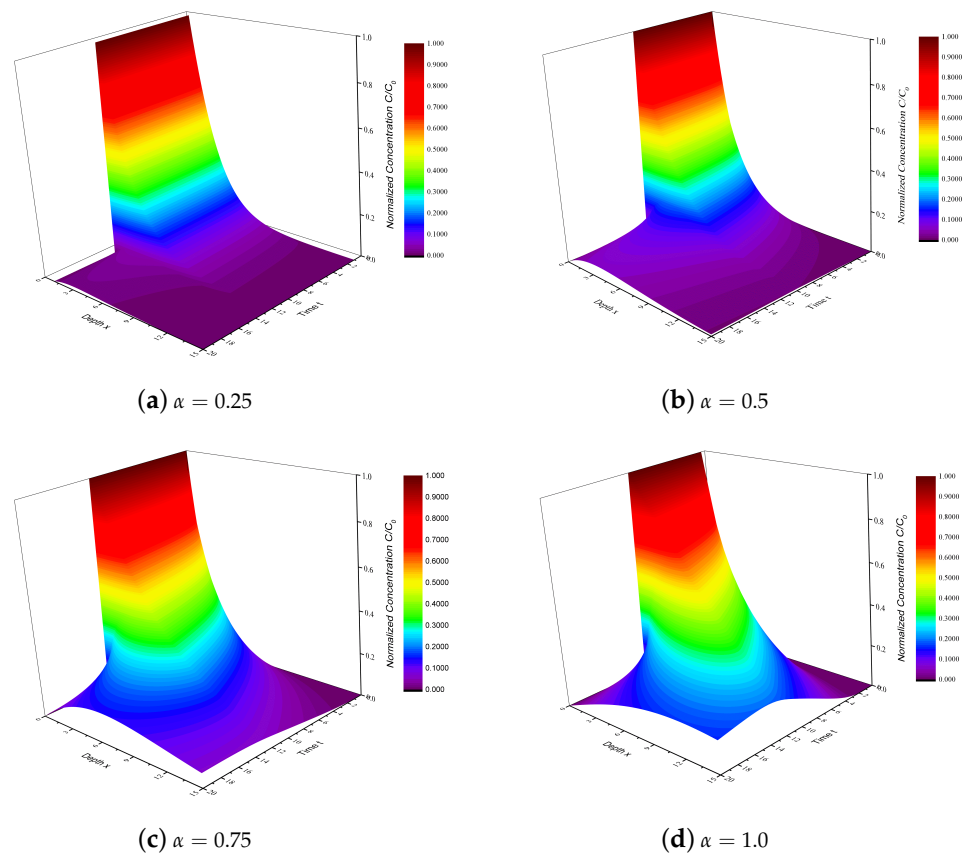


Figure 1. Concentration distribution of AB-ADM with linear adsorption in Equation (11) with different α values when $D_\alpha, u = 0.01, R = 2, t_0 = 12, C_0 = 1$.

For the limit of time t_0 , cases for different concentration sources can be derived.

3.1. AB-ADM with Linear Adsorption for Pulse-like Input Source

When $t_0 \rightarrow 0$, $C(0, t) = C_0 \delta(t)$, it develops into

$$\begin{cases} {}^{AB}D_t^\alpha [C_\delta(x, t)] = \frac{D_\alpha}{R} \frac{\partial^2 C_\delta(x, t)}{\partial x^2} - \frac{u}{R} \frac{\partial C_\delta(x, t)}{\partial x} \\ C_\delta(0, t) = C_0 \delta(t), C_\delta(\infty, t) = 0, C_\delta(x, 0) = 0, \frac{\partial C_\delta}{\partial x} \Big|_{x=\infty} = 0 \end{cases} \quad (12)$$

Through a similar process of calculation, the exact solution to Equation (12) can be represented as

$$C_\delta(x, t) = \frac{2C_0 D_\alpha}{\pi R} \exp\left(\frac{ux}{2D_\alpha}\right) \int_0^\infty B\xi \left[(1 - \alpha)\delta(t) + \alpha Bt^{\alpha-1} E_{\alpha, \alpha}(-At^\alpha) \right] \sin(\xi x) d\xi. \quad (13)$$

When $\alpha = 1$, Equation (13) is reduced to

$$\begin{aligned} C_\delta(x, t) &= \frac{2C_0D}{\pi R} \exp\left(\frac{ux}{2D}\right) \exp\left(-\frac{u^2t}{4DR}\right) \int_0^\infty \xi \exp\left(-\frac{D\xi^2t}{R}\right) \sin(\xi x) d\xi \\ &= \frac{C_0x}{2} \sqrt{\frac{R}{\pi Dt^3}} \exp\left[-\frac{(Rx - ut)^2}{4DRt}\right]. \end{aligned} \quad (14)$$

Figure 2 indicates that the suggested model in Equation (13) fits the experimental data [45] well and is appropriate to describe advection dispersion problems. The numerical simulations of the AB-ADM in Equation (13) for different α values are displayed in Figure 3.

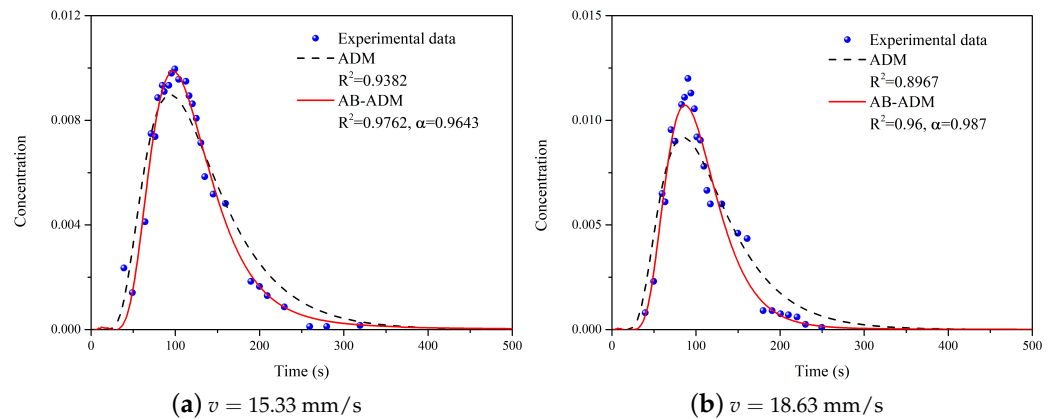


Figure 2. Fits of breakthrough profiles for different average-flow velocity values [45] using AB-ADM in Equation (13) and ADM in Equation (14).

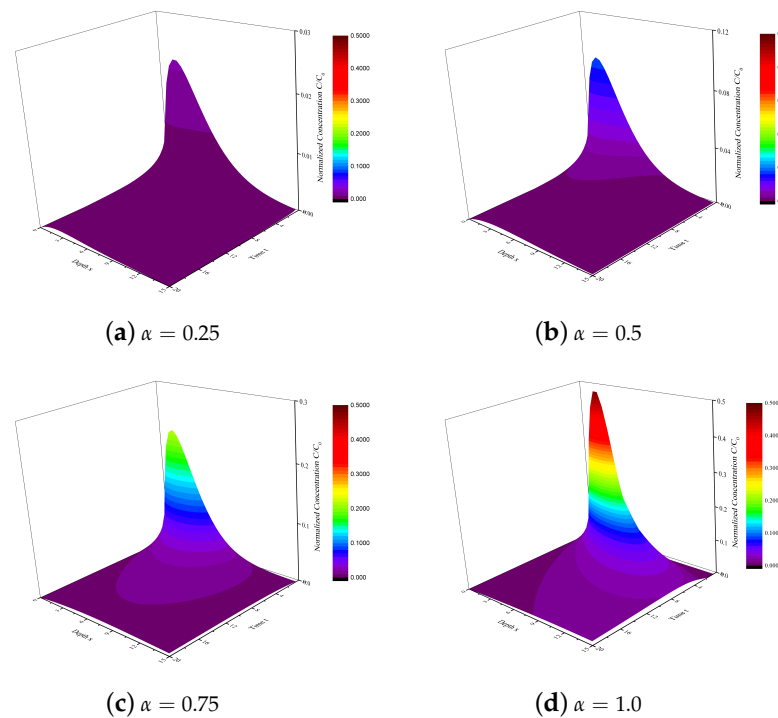


Figure 3. Concentration distributions of AB-ADM with linear adsorption for an instantaneous concentration source in Equation (13) with different α values when $D_\alpha = 10$, $u = 0.01$, $R = 2$, $C_0 = 1$.

3.2. AB-ADM with Linear Adsorption for Constant Concentration Source

When $t_0 \rightarrow \infty$, $C(0, t) = C_0$, it comes to

$$\begin{cases} {}^ABD_t^\alpha [C_c(x, t)] = \frac{D_\alpha}{R} \frac{\partial^2 C_c(x, t)}{\partial x^2} - \frac{u}{R} \frac{\partial C_c(x, t)}{\partial x} \\ C_c(0, t) = C_0, C_c(\infty, t) = 0, C_c(x, 0) = 0, \frac{\partial C_c}{\partial x} \Big|_{x=\infty} = 0 \end{cases} \quad (15)$$

Further, the exact analytic solution of the AB-ADM in Equation (15) is

$$C_c(x, t) = C_0 - \frac{2}{\pi} C_0 \exp\left(\frac{ux}{2D_\alpha}\right) \int_0^\infty \frac{\xi B}{\xi^2 + \frac{u^2}{4D_\alpha^2}} E_\alpha(-At^\alpha) \sin(\xi x) d\xi. \quad (16)$$

When $\alpha = 1$, Equation (16) can be presented as

$$\begin{aligned} C_c(x, t) &= C_0 \left\{ 1 - \frac{1}{2} \left[\operatorname{erfc}\left(\frac{ut - Rx}{2\sqrt{D_\alpha R t}}\right) - \exp\left(\frac{ux}{D_\alpha}\right) \operatorname{erfc}\left(\frac{ut + Rx}{2\sqrt{D_\alpha R t}}\right) \right] \right\} \\ &= \frac{1}{2} C_0 \left[\operatorname{erfc}\left(\frac{Rx - ut}{2\sqrt{D_\alpha R t}}\right) + \exp\left(\frac{ux}{D_\alpha}\right) \operatorname{erfc}\left(\frac{Rx + ut}{2\sqrt{D_\alpha R t}}\right) \right]. \end{aligned} \quad (17)$$

which is the asymmetrical solution to the classical ADM proposed by Ogata and Banks [46].

Figure 4 indicates that the AB-ADM in Equation (16) fits the experimental data better than the classical ADM in Equation (17). The numerical simulations of the AB-ADM in Equation (16) are exhibited in Figure 5.

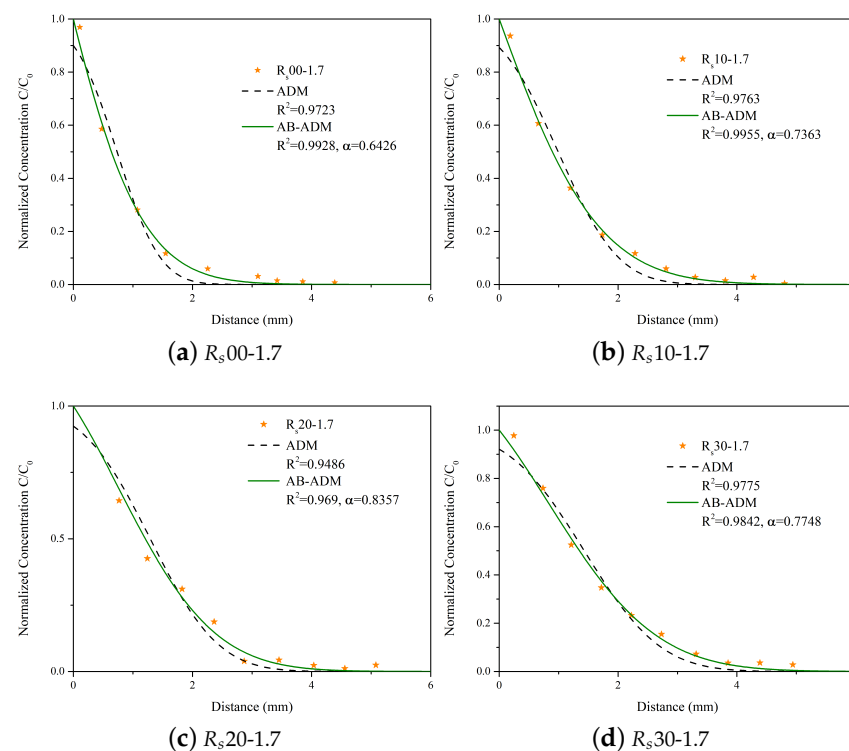


Figure 4. Cont.

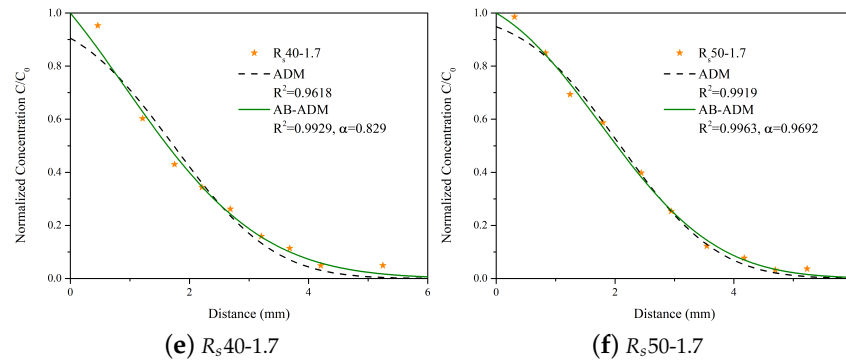


Figure 4. Fits of breakthrough profiles for Eu(III) in compacted mixtures with different R_s after 300 days [47] via AB-ADM in Equation (16) and ADM in Equation (17).

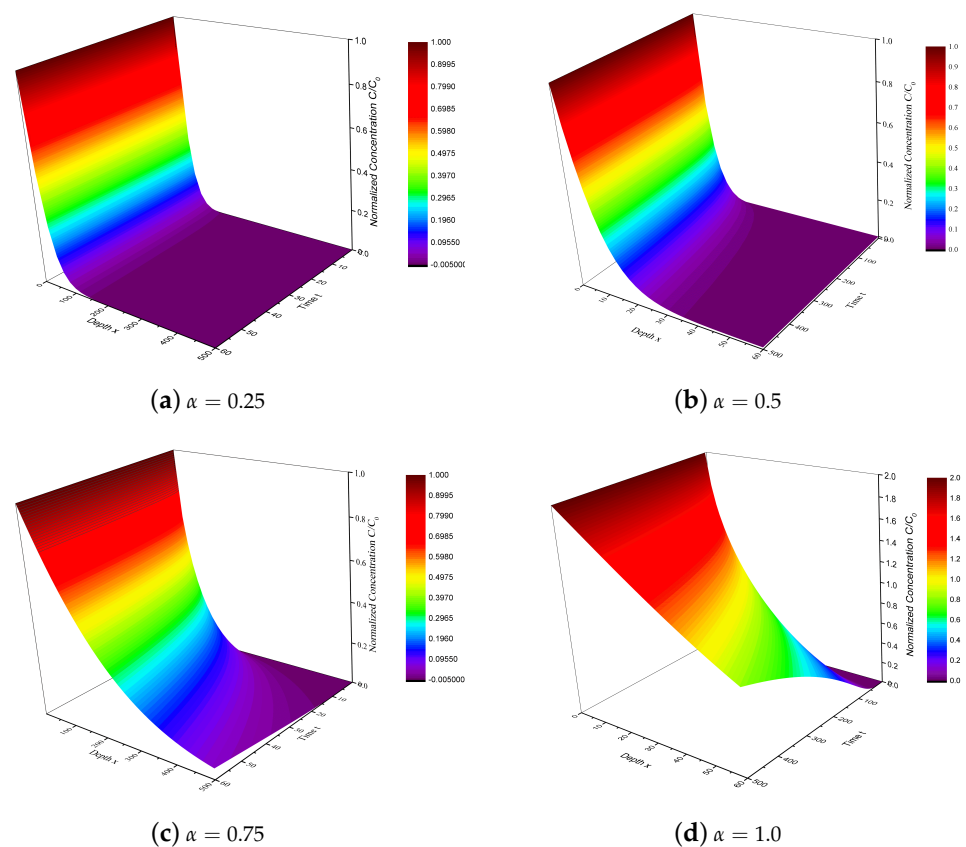


Figure 5. Numerical simulations of AB-ADM with linear adsorption for a constant concentration source in Equation (16) with different α values when $D_\alpha = 10$, $u = 0.01$, $R = 2$, $C_0 = 1$.

4. The AB-ADM with First-Order Decay

If it is assumed that the contaminant transport is subject to first-order decay without multi-step or nonlinear reactions, then the sinks or source term is

$$R_s(x, t) = -\lambda C(x, t), \quad (18)$$

where λ is the decay constant.

Integrating Equation (18) into Equation (3) results in

$${}_0^{\text{AB}}D_t^\alpha [C(x, t)] = D_\alpha \frac{\partial^2 C(x, t)}{\partial x^2} - u \frac{\partial C(x, t)}{\partial x} - \lambda C(x, t). \quad (19)$$

Introducing the new function $H(x, t)$ satisfied $C(x, t) = H(x, t) \exp(\frac{ux}{2D_\alpha})$, and making use of F.S.T. and L.T. with Equation (19) develops into

$$\tilde{H}(\xi, s) = [1 - \exp(-st_0)]\tilde{H}_1(\xi, s), \quad (20)$$

where

$$\tilde{H}_1(\xi, s) = \sqrt{\frac{2}{\pi}} C_0 D_\alpha \xi G \left[(1 - \alpha) \frac{s^{\alpha-1}}{s^\alpha + K} + \alpha \frac{s^{-1}}{s^\alpha + K} \right], \quad (21)$$

$G = \frac{1}{1 + (1 - \alpha)(D_\alpha \xi^2 + \frac{u^2}{4D_\alpha} + \lambda)}$, $K = \frac{\alpha(D_\alpha \xi^2 + \frac{u^2}{4D_\alpha} + \lambda)}{1 + (1 - \alpha)(D_\alpha \xi^2 + \frac{u^2}{4D_\alpha} + \lambda)}$; employing I.F.S.T. and inverse L.T. to Equation (21) results in

$$H_1(x, t) = C_0 \exp\left(-\frac{Nx}{2D_\alpha}\right) - \frac{2}{\pi} C_0 \int_0^\infty \frac{\xi G}{\xi^2 + \frac{N^2}{4D_\alpha^2}} E_\alpha(-Kt^\alpha) \sin(\xi x) d\xi, \quad (22)$$

where $N = \sqrt{u^2 + 4D_\alpha \lambda}$.

Further, when I.F.S.T. and inverse L.T. are employed with Equation (20), considering Equations (A3) and (22), the exact solution of Equation (19) is

$$C(x, t) = H(x, t) \exp(\frac{ux}{2D_\alpha}) = \begin{cases} C_2(x, t) & 0 < t \leq t_0 \\ C_2(x, t) - C_2(x, t - t_0) & t_0 < t < +\infty \end{cases}, \quad (23)$$

where $C_2(x, t) = C_0 \exp\left(\frac{u-N}{2D_\alpha}x\right) - \frac{2}{\pi} C_0 \exp\left(\frac{ux}{2D_\alpha}\right) \int_0^\infty \frac{\xi G}{\xi^2 + \frac{N^2}{4D_\alpha^2}} E_\alpha(-Kt^\alpha) \sin(\xi x) d\xi$.

Figure 6 shows concentration distributions of AB-ADM with first-order decay in Equation (23) for different fractional index α values.

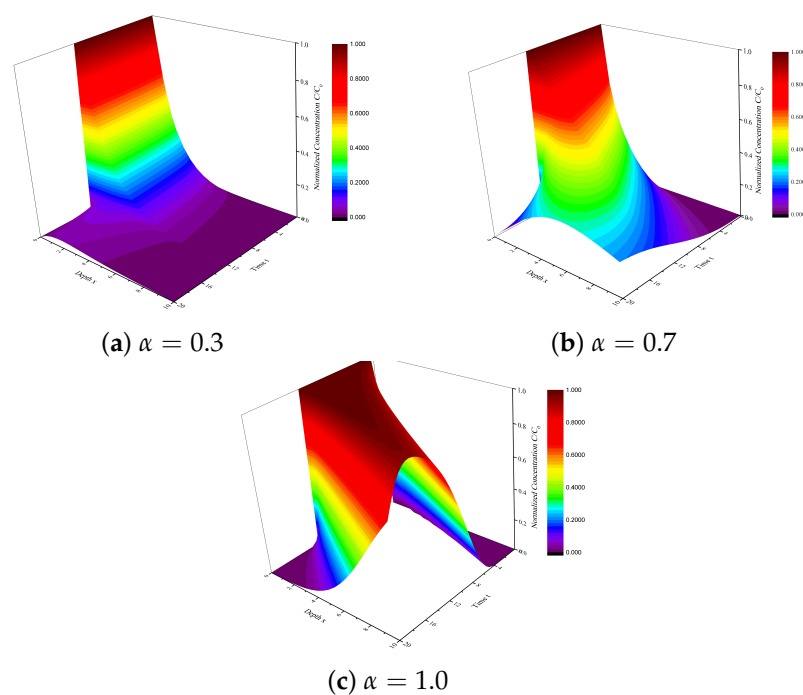


Figure 6. Numerical simulations of AB-ADM with first-order decay in Equation (23) with different α values when $D_\alpha = 0.5$, $u = 1$, $\lambda = 10^{-4}$, $t_0 = 12$, $C_0 = 1$.

It is easy to infer that the hypothesis of a constant source case is valid for a large enough time, t_0 . When $t_0 \rightarrow \infty$, it comes to

$$\begin{cases} {}^AB D_t^\alpha [C_c(x, t)] = D_\alpha \frac{\partial^2 C_c(x, t)}{\partial x^2} - u \frac{\partial C_c(x, t)}{\partial x} - \lambda C_c(x, t) \\ C_c(0, t) = C_0, C_c(\infty, t) = 0, C_c(x, 0) = 0, \frac{\partial C_c}{\partial x} \Big|_{x=\infty} = 0 \end{cases} \quad (24)$$

Similarly, the analytical solution of AB-ADM in Equation (24) is

$$C_c(x, t) = C_0 \exp\left(\frac{u - N}{2D_\alpha} x\right) - \frac{2}{\pi} C_0 \exp\left(\frac{ux}{2D_\alpha}\right) \int_0^\infty \frac{\xi G}{\xi^2 + \frac{N^2}{4D_\alpha^2}} E_\alpha(-Kt^\alpha) \sin(\xi x) d\xi. \quad (25)$$

When $\alpha = 1$,

$$\begin{aligned} & \frac{C_c(x, t)}{C_0} \\ &= \exp\left(\frac{u - N}{2D} x\right) - \frac{2}{\pi} \exp\left(\frac{ux}{2D}\right) \int_0^\infty \frac{\xi}{\xi^2 + \frac{N^2}{4D^2}} \left\{ 1 - \exp\left[-Dt\left(\xi^2 + \frac{N^2}{4D^2}\right)\right] \right\} \sin(\xi x) d\xi \\ &= \exp\left(\frac{u - N}{2D} x\right) - \frac{1}{2} \left[\exp\left(\frac{u - N}{2D} x\right) \operatorname{erfc}\left(\frac{Nt - x}{2\sqrt{Dt}}\right) - \exp\left(\frac{u + N}{2D} x\right) \operatorname{erfc}\left(\frac{Nt + x}{2\sqrt{Dt}}\right) \right] \\ &= \frac{1}{2} \left[\exp\left(\frac{u - N}{2D} x\right) \operatorname{erfc}\left(\frac{x - Nt}{2\sqrt{Dt}}\right) + \exp\left(\frac{u + N}{2D} x\right) \operatorname{erfc}\left(\frac{x + Nt}{2\sqrt{Dt}}\right) \right], \end{aligned} \quad (26)$$

the classical symmetric analytical solution of ADM [48] is acquired.

Figure 7 indicates that the fitting results of AB-ADM in Equation (25) with experimental data [49] for long-term tritium transport are better than the fitting results of ADM in Equation (26). The numerical simulations of the AB-ADM in Equation (25) are displayed in Figure 8.

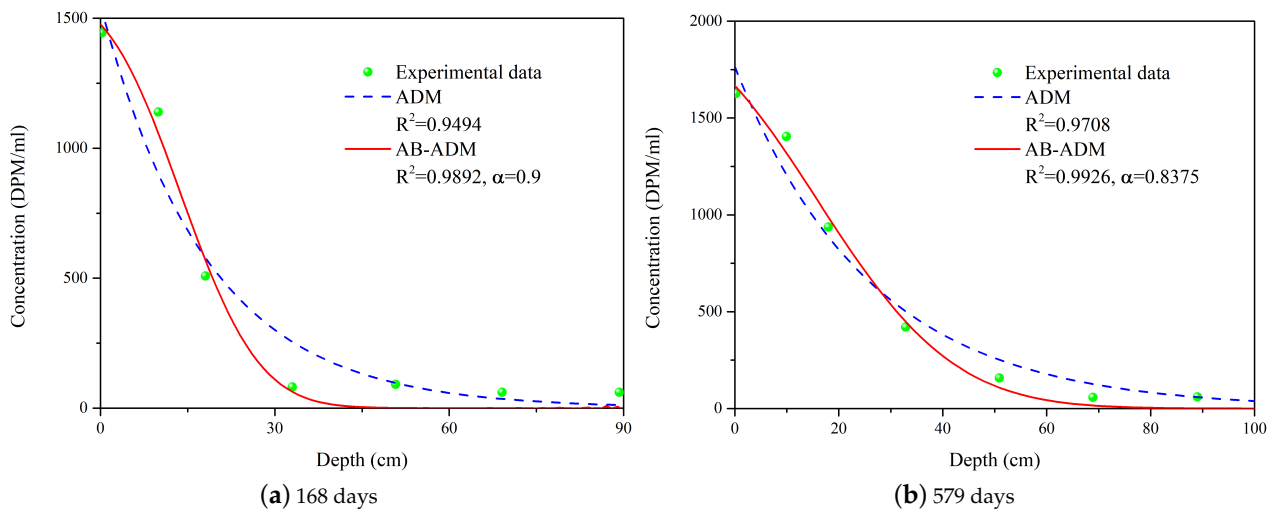


Figure 7. Fits of breakthrough profiles for tritium transport [49] via AB-ADM in Equation (25) and ADM in Equation (26).

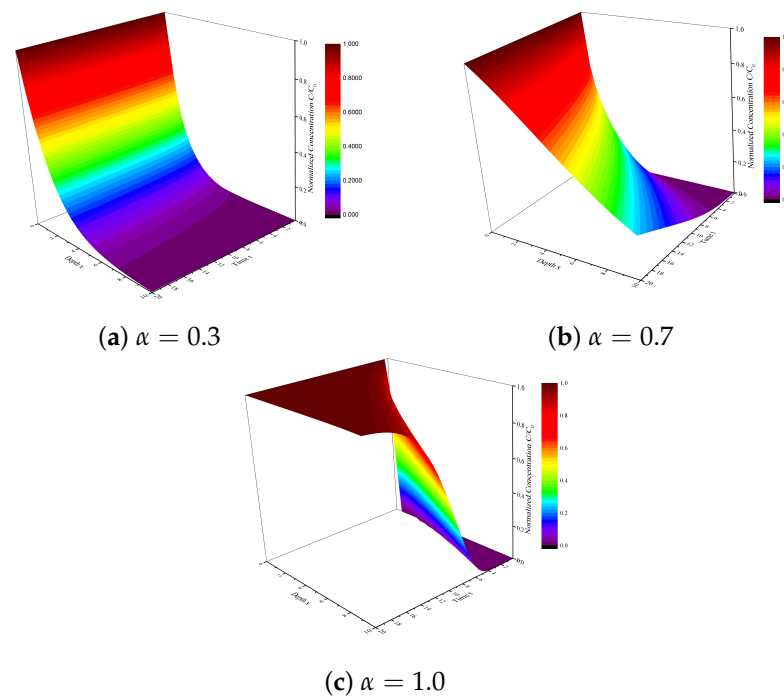


Figure 8. Numerical simulations of AB-ADM with first-order decay for constant source in Equation (25) with different α values when $D_\alpha = 0.5$, $u = 1$, and $\lambda = 10^{-4}$, $C_0 = 1$.

5. Discussion

In this work, the AB differential operator is introduced to the ADM to describe contaminant transport in geological systems. The exact analytic solutions of the new models are given in the light of two cases, including adsorption and first-order decay. The results of the experimental data-fitting analysis indicate that the fractional models provide a relatively more accurate fit. The classical ADMs are demonstrated to be the particular limiting cases of the suggested models. The AB-ADM could be applied to the process of laboratory columns, radionuclide migration, and groundwater solute transport. However, the proposed models still face limitations. Firstly, AB-ADM with linear adsorption neglects nonlinear sorption isotherms (like Freundlich and Langmuir), which are often observed in soils and rocks; this limits applicability. Secondly, the proposed models only considered the first-order decay, which is simplistic, but many contaminants undergo high-order decay or nonlinear reactions, which should also be taken into account. Thirdly, the boundary conditions are somehow idealized for contaminant transport in real geological systems. In addition, the fractional parameter α represents the power-law or memory effect in the contaminant transport process, we should further discuss and address its physical meaning. Whether it is linked to pore-scale heterogeneity, memory in adsorption, or anomalous diffusion pathways certainly needs to be validated in further investigations. The AB-ADM with first-order decay is compared with tritium transport data, but long-term predictions and deviations at later times are not analyzed. The benchmarking against other fractional or stochastic models (Caputo-based ADE, continuous-time random walk) is lacking. The presented AB-ADM should help assess and compare different formulations of contaminant transport models in describing anomalous diffusion dynamics. Moreover, different forms of crossovers to normal dynamics should be studied. For practical application in contaminant transport, the most significance is extending AB-ADMs to two- or three-dimensional cases incorporating variable velocity fields, nonlinear sorption, and reactive transport coupling, which would better reflect the natural geological systems. In order to accomplish these generalizations, undertaking an effective (convergent and stable), a numerical simulation

is also required. All of these further studies would improve the applicability of AB-ADM and help engineers or hydrogeologists predict contaminant spread more reliably.

6. Conclusions

The AB-ADMs using the AB differential operator are more capable of catching the concentration variation characteristics presented in the real-world experimental data than the traditional ADMs from the data-based fitting results. The AB-ADMs provides flexible and adequate simulations of contaminant transport by selecting different differential-order α values. Towards the end, all the results are supported with the assistance of graphical portrayal via a numerical investigation, which would be beneficial for researchers to contemplate the dynamics of the contaminant transport. As a consequence, the proposed AB-ADM provide an effective description of contaminant transport in a geological environment.

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Abbreviations

The following abbreviations are used in this manuscript:

ADM	Advection–dispersion model
AB	Atangana–Baleanu
AB-ADMs	Atangana–Baleanu advection-dispersion models
L.T.	Laplace transform
I.L.T.	Inverse Laplace transform
F.S.T.	Fourier sine transform
I.F.S.T.	Inverse Fourier sine transform

Appendix A. Integral Transforms

We give the basic mathematical formula used in the calculation process. The Laplace transform (L.T) [43] of $g(t)$ is defined as

$$\mathcal{L}[g(t)] = \int_0^{\infty} g(t) \exp(-st) dt. \quad (\text{A1})$$

In addition, we recall some L.T. of basic functions herein that will be used later in this work [31,43]:

$$\mathcal{L}\left\{{}_0^{AB}D_t^\alpha[g(t)]\right\} = \frac{s^\alpha \mathcal{L}\{g(t)\} - s^{\alpha-1}g(0)}{(1-\alpha)s^\alpha + \alpha}, \quad (\text{A2})$$

$$\mathcal{L}[g(t - \tau)] = \exp(-s\tau)\mathcal{L}[g(t)], \quad (\text{A3})$$

$$\mathcal{L}\left\{t^{\beta-1}E_{\alpha,\beta}(\pm at^{\alpha})\right\} = \frac{s^{\alpha-\beta}}{s^{\alpha} \mp a}, a \in \mathbb{R}. \quad (\text{A4})$$

$$\mathcal{L}[\varepsilon(t - a)] = \frac{1}{s} \exp(-as). \quad (\text{A5})$$

The Fourier sine transform (F.S.T.) [50] of $g(x)$ is

$$F_s[g(x)] = \sqrt{\frac{2}{\pi}} \int_0^{\infty} g(x) \sin(\xi x) dx, \quad (\text{A6})$$

and the inverse Fourier sine transform (I.F.S.T.) of $F_s(\xi)$ is $g(x) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} F_s(\xi) \sin(\xi x) d\xi$.
The properties of F.S.T. are as follows,

$$F_s\{g''(x)\} = -\xi^2 F_s(\xi) + \sqrt{\frac{2}{\pi}} g(0)\xi, \text{ where } g(\infty) = 0, g'(\infty) = 0. \quad (\text{A7})$$

$$F_s\{\exp(-px)\} = \sqrt{\frac{2}{\pi}} \frac{\xi}{\xi^2 + p^2}, \quad (\text{A8})$$

$$F_s\left\{\exp(-bx)\operatorname{erfc}\left(ab - \frac{x}{2a}\right) - \exp(bx)\operatorname{erfc}\left(ab + \frac{x}{2a}\right)\right\} = \sqrt{\frac{2}{\pi}} \frac{2\xi}{\xi^2 + b^2} \exp[-a^2(\xi^2 + b^2)]. \quad (\text{A9})$$

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