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ANALYTIC SOLUTION OF FRACTIONAL ADVECTION DISPERSION EQUATION WITH DECAY FOR CONTAMINANT TRANSPORT IN POROUS MEDIA

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Abstract. Advection and dispersion are the movements of contaminants/solute particles along with flowing groundwater at the seepage velocity in porous media. The aim of this paper is to find concentration of contaminant in flowing groundwater using fractional advection dispersion equation with decay involving Hilfer derivative with respect to time. Time fractional advection-dispersion equation describe particle's motion with memory in time. The solution of time fractional advection dispersion equation with decay is obtained in terms of Mittag-Leffler function and Green function. The effect of the decay is to reduce mass and concentration of the solution, which is a function of time and space variable.

1. Introduction

Groundwater hydrology may be defined as the science of the occurrence, distribution and flow of the ground water below the surface of the earth. Groundwater contamination usually occurs by natural or man made resources. The contaminants enter in the groundwater system from the land surface by seawater intrusion.

Groundwater composition may be changed due to natural process by evapotranspiration, percolation of chemicals in groundwater (chlorides, sulphates, nitrates, fluoride, arsenic), radioactive elements etc. Also, man made products and waste are the sources of the groundwater contamination. Groundwater contamination also occurs by spills and leaks, agricultural products, mining, saltwater, acid rain, surface water, improper well construction, maintenance etc.

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2. Mathematical model

Advection - dispersion is the transport process of groundwater contaminants. Advection is the movement of contaminants along with flowing groundwater at the seepage velocity in porous media and dispersion is a process caused by velocity variations in the porous media. The derivation of the advection dispersion equation for solute transport is derived from the law of conservation of mass. The derivation of advection dispersion equation is presented in [4].

We consider that the medium is homogeneous and isotropic, the flow is in nonsteady state and the Darcy's law applies. The flow is described by the seepage velocity, which transports the dissolved substance by advection. There is an additional mixing process, hydrodynamic dispersion, which is caused by velocity variations within groundwater flow.



Figure 1: Mass balance in a cubic element in space

Figure 1 shows the solute flux into and out of a representative volume in the porous medium. The velocity v has components v_x, v_y, v_z and the seepage velocity $\bar{v} = \frac{v}{n}$, n being effective porosity of the porous medium, has components $\bar{v}_x, \bar{v}_y, \bar{v}_z$.

In the x direction, the mass of solute transported is given as

Transport by advection
$$= \bar{v}_x nC \, dA$$
,
 ∂C

Transport by dispersion
$$= n \mathcal{D}_x \frac{\partial \mathcal{D}}{\partial x} dA$$
,

where \mathcal{D}_x is the dispersion coefficient and dA is the cross section area of cubic element. Governing equation of solute concentration C = C(x, y, z, t) in three dimensions is

$$\frac{\partial C}{\partial t} = -\left[v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + v_z \frac{\partial C}{\partial z}\right] + \left[\mathcal{D}_x \frac{\partial^2 C}{\partial x^2} + \mathcal{D}_y \frac{\partial^2 C}{\partial y^2} + \mathcal{D}_z \frac{\partial^2 C}{\partial z^2}\right].$$
 (1)

In one dimension, (1) reduces to

$$\frac{\partial C(x,t)}{\partial t} = -v \frac{\partial C(x,t)}{\partial x} + \mathcal{D} \frac{\partial^2 C(x,t)}{\partial x^2},\tag{2}$$

where initial and boundary conditions depend on the type of the model. Here C is the solute concentration, t(> 0) is the time, $x \in \mathbb{R}$ is the soil depth, v(> 0) is the seepage velocity and $\mathcal{D}(> 0)$ is the dispersion coefficient.

Bastian and Lapidus, Banks and Ali, Ogata, Marino, Al-Niami and Rushton, Singh et al. solved the advection dispersion equation (2) for different initial conditions analytically, to predict the contaminant concentration distribution along and against transient groundwater flow in finite aquifer.

Analytic solutions of generalized one dimensional advection-dispersion equation were also obtained by adding some variable or constant term in equation (2). Robert [16] got an exact analytical solution to the advection-dispersion equation with decay coefficient subject to a continuous load of finite duration. Mazaheri et al. [9] presented the analytical solution of the one dimensional advection dispersion equation with different initial and boundary conditions.

Analytic solutions of fractional advection dispersion equation are obtained by many authors for equation (2) by fractionalizing the integer order derivatives with respect to time and space variables. Liu et al. [7] derived complete solution of the time fractional advection dispersion equation of order α using integral transform methods, where the first-order derivative with respect to time was replaced by Caputo fractional derivative. Tariq and Ahmad [18] obtained exact solution of the time fractional advection dispersion equation with decay. Schumer et al. [17] obtained solutions of fractional advection dispersion equation by various approaches. Benson et al. [2] derived the solution for the multidimensional advection and fractional dispersion equation. Benson et al. [1] emphasized that fractional derivatives come from the governing equations of stable Levy motion. They discussed the Eulerian and Lagrangian numerical solutions for solving fractional partial differential equations. These numerical approximations are nearly as robust as proven methods for classical diffusion. Eulerian approximations has been proven stable for the fractional advection dispersion equation. Recently, Schumer et al. [17] have derived results using fractional order derivatives which give better prediction of groundwater flow problems when compared to the experimental data.

In this paper, we present analytic solution of the one-dimensional advection dispersion equation, fractionalized with respect to time variable using Hilfer derivative which is more general in nature than Caputo and Riemann-Liouville derivatives. So, it provides unification and generalization of the already existing results. We consider the following time fractional advection-dispersion equation

$$D_0^{\mu,\rho}(C(x,t)) = -v \frac{\partial C(x,t)}{\partial x} + \mathcal{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \lambda C(x,t),$$

$$0 < \mu \le 1, \ 0 \le \rho \le 1, \ t > 0, \ x \in (-\infty,\infty),$$
(3)

where $\lambda \ge 0$ is the first order decay rate and the source of contamination is unknown. The decay could be caused by radioactive decay, biodegradation or hydrolysis.

In equation (3) if we take $\lambda = 0$, we get generalized time fractional advection dispersion equation. We shall make use of Laplace transform for time variable and Fourier transform for space variable as the source of contamination is unknown.

3. Mathematical preliminaries

Let $\operatorname{Re}(\rho) > 0$ and f be piecewise continuous on interval $J' = (0, \infty)$ and integrable on any finite subinterval of $J = [0, \infty)$. Then

$$\left(I_{a+}^{\rho}f\right)(t) = \left({}^{RL}D_{a+}^{-\rho}f\right)(t) = \frac{1}{\Gamma(\rho)}\int_{a}^{t}(t-\xi)^{\rho-1}f(\xi)\,d\xi,\ t>0,$$

is called the Riemann-Liouville fractional integral [8, Eq. 2.2, p. 45] of order $\rho,$ and

$$\binom{RL}{a} D_{a+f}^{\rho}(t) = \left(\frac{d}{dt}\right)^{m+1} \frac{1}{\Gamma(\rho)} \int_{a}^{t} (t-\xi)^{m-\rho} f(\xi) \, d\xi, \quad m \le \rho < (m+1),$$
(4)

is called the Riemann-Liouville fractional derivative of order ρ [8, Eq. 2.1, p. 82].

Caputo's definition [3, Eq. 5, p. 530] of fractional derivative of $f : [a, b] \to \mathbb{R}$ of order ρ is given by

$${}^{C}D_{a+}^{\rho}f(t) = \begin{cases} \frac{1}{\Gamma(\rho-n)} \int_{a}^{t} \frac{f^{(n)}(\tau) d\tau}{(t-\tau)^{\rho+1-n}}, & (n-1) < \rho < n, \\ \frac{d^{n}f(t)}{dt^{n}}, & \rho = n. \end{cases}$$

REMARK 3.1. In Riemann-Liouville fractional derivative, the function need not be continuous and/or differentiable at the origin. Riemann-Liouville fractional derivative has some disadvantages when trying to solve model real-world problems which reduce its applicability in the field. The Caputo derivative allows initial and boundary conditions to be included in the formulation of the problem when dealing with real-world problems.

Hilfer [6] studied a generalized fractional operator having the Riemann-Liouville and the Caputo derivatives as its particular cases. Hilfer derivative of order μ and type ρ with respect to time t is defined as

$$D_{a+}^{\mu,\rho}f(t) = \left(I_{a+}^{\rho(1-\mu)}\frac{d}{dt}\left(I_{a+}^{(1-\mu)(1-\rho)}f\right)\right)(t), \quad 0 < \mu \le 1, \ 0 \le \rho \le 1,$$
(5)

where $I_{a+}^{\rho(1-\mu)}$ and $I_{a+}^{(1-\mu)(1-\rho)}$ are the Riemann-Liouville fractional integral operators of order $\rho(1-\mu)$ and $(1-\mu)(1-\rho)$, respectively.

Definition (5) reduces to the Riemann-Liouville fractional derivative for $\rho = 0$, and for $\rho = 1$, it reduces to the Caputo fractional derivative.

Laplace transformation of Hilfer derivative of f in equation (5) was given by Tomovski [20, Eq. 1.5] in the following form:

$$L\{D_{a+}^{\mu,\rho}f(t)\}(u) = u^{\mu}L\{f(t)\}(u) - u^{\rho(\mu-1)} \Big(I_{a+}^{(1-\mu)(1-\rho)}f\Big)(0), \operatorname{Re}(\mu) > 0, \operatorname{Re}(\rho) > 0, (6)$$

where the initial value $\left(I_{a+}^{(1-\mu)(1-\rho)}f\right)(0)$ is the Riemann-Liouville integral of f evaluated in the limit as $t \to 0$.

The Mittag-Leffler function $E_{\alpha,\beta}$ is a special function obtained by generalizing the definition of exponential function. Its importance is realized due to its direct involvement in the problems of physics, biology, engineering and applied sciences. Mittag-Leffler function is useful to find the solution of fractional order differential and integral equations.

One parameter Mittag-Leffler function was given by Mittag-Leffler [10] as

$$E_{\alpha}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha+1)}, \quad \operatorname{Re}(\alpha) > 0, \ \alpha \in \mathbb{C}, \ z \in \mathbb{C}.$$

Two parameters Mittag-Leffler function is defined by Wiman [21] as

$$E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + \beta)}, \quad \operatorname{Re}(\alpha) > 0, \ \operatorname{Re}(\beta) > 0, \ \alpha, \beta \in \mathbb{C}, \ z \in \mathbb{C}.$$

The series converges for all values of the argument $z \in \mathbb{C}$, so the Mittag-Leffler function is an entire function.

4. Time fractional advection dispersion equation

In this section we derive the solution of one dimensional time fractional advection dispersion equation with decay by applying Fourier transform and Laplace transform.

$$D_0^{\mu,\rho}C(x,t) = -v \frac{\partial C(x,t)}{\partial x} + \mathcal{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \lambda C(x,t), \quad x \in (-\infty,\infty), \ t > 0$$
(7)

with initial and boundary conditions

$$I_0^{(1-\mu)(1-\rho)}C(x,0) = f(x), \quad 0 < \mu \le 1, \ 0 \le \rho \le 1,$$
(8)

$$\lim_{|x| \to \infty} C(x, t) = 0, \quad t > 0,$$
(9)

where $D_0^{\mu,\rho}$ is the Hilfer derivative. $I_0^{(1-\mu)(1-\rho)}C(x,0)$ is the Riemann-Liouville fractional integral operator of order $(1-\mu)(1-\rho)$. C(x,t) is concentration of solute and f(x) is the real valued function. Then the solution of equation (7) is given by

$$C(x,t) = \int_{-\infty}^{\infty} G(x-y,t)f(y) \, dy,$$

$$G(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\mu+\rho(1-\mu)} [(ivk - \lambda + k^2)t^{\mu}] e^{-ikx} \, dk$$

where

is the Green's function.

Proof. We take the Fourier transform of equation (7) w.r.t. space variable x as

$$D_0^{\mu,\rho}(C^*(k,t)) = ivkC^*(k,t) + \mathcal{D}k^2C^*(k,t) - \lambda C^*(k,t),$$
(10)

where $C^*(k, t)$ is the Fourier transform of function C(x, t). Now we take Laplace transform of equation (10) w.r.t. time variab

Now we take Laplace transform of equation (10) w.r.t. time variable t and use equation (6); we obtain

$$s^{\mu}\tilde{C}^{*}(k,s) - s^{\rho(\mu-1)}I_{0}^{(1-\mu)(1-\rho)}C(k,0)$$

= $ivk\tilde{C}^{*}(k,s) + \mathcal{D}k^{2}\tilde{C}^{*}(k,s) - \lambda\tilde{C}^{*}(k,s), \operatorname{Re}(s) > 0.$ (11)

Taking the Fourier transform of the initial condition (8), we get $F\{I_0^{(1-\mu)(1-\rho)}f(x)\}(k) = f^*(k)$. Therefore, equation (11) becomes

$$(s^{\mu} - ivk - \mathcal{D}k^{2} + \lambda)\tilde{C}^{*}(k, s) = s^{\rho(\mu-1)}f^{*}(k) \Rightarrow \tilde{C}^{*}(k, s) = \frac{s^{\rho(\mu-1)}f^{*}(k)}{s^{\mu} - ivk - \mathcal{D}k^{2} + \lambda}.$$
 (12)

Taking inverse Laplace transform of equation (12) and using the following result by Haubold et al. [5, Eq. 18]

$$L^{-1}\left(\frac{s^{\beta-1}}{s^{\alpha}+a}\right) = t^{\alpha-\beta}E_{\alpha,\,\alpha-\beta+1}(-at^{\alpha}), \text{ Re}(s) > 0, \text{ Re}(\alpha) > 0, \text{ Re}(\alpha-\beta) > -1,$$

we obtain

$$C^{*}(k,t) = t^{\mu+\rho(1-\mu)-1} E_{\mu,\ \mu+\rho(1-\mu)} [(-\lambda + ivk + \mathcal{D}k^{2})t^{\mu}] f^{*}(k).$$
(13)

Taking inverse Fourier transform of equation (13), w.r.t. k we get

$$\begin{split} C(x,t) &= \frac{t^{\mu+\rho(1-\mu)-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\ \mu+\rho(1-\mu)} [(-\lambda+ivk+\mathcal{D}k^2)t^{\mu}] e^{-ikx} f^*(k) \, dk \\ &= \frac{t^{\mu+\rho(1-\mu)-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\ \mu+\rho(1-\mu)} [(-\lambda+ivk+\mathcal{D}k^2)t^{\mu}] e^{-ikx} \int_{-\infty}^{\infty} e^{iky} f(y) \, dy \, dk \\ &= \int_{-\infty}^{\infty} \left(\frac{t^{\mu+\rho(1-\mu)-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\ \mu+\rho(1-\mu)} [(-\lambda+ivk+\mathcal{D}k^2)t^{\mu}] e^{-ik(x-y)} \, dk \right) f(y) \, dy \\ &= \int_{-\infty}^{\infty} G(x-y,t) f(y) \, dy, \end{split}$$

is the formal solution of equation (7), where

$$G(x,t) = \frac{t^{\mu+\rho(1-\mu)-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\ \mu+\rho(1-\mu)} [(-\lambda+ivk+\mathcal{D}k^2)t^{\mu}] e^{-ikx} \, dk.$$

is the Green function.

5. Special cases

By giving particular values to different parameters, a number of special cases can be obtained.

1. Consider $\lambda = 0$; then Theorem 4.1 becomes

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THEOREM 5.1. Consider the time fractional advection dispersion equation

$$D_0^{\mu,\rho}C(x,t) = -v \,\frac{\partial C(x,t)}{\partial x} + \mathcal{D} \,\frac{\partial^2 C(x,t)}{\partial x^2}, \quad x \in (-\infty,\infty), \ t > 0 \tag{14}$$

with initial and boundary conditions

$$I_0^{(1-\mu)(1-\rho)}C(x,0) = f(x), \quad 0 < \mu < 1, \ 0 \le \rho \le 1, \quad \lim_{|x| \to \infty} C(x,t) = 0,$$

where $D_0^{\mu,\rho}$ is the Hilfer derivative, $I_0^{(1-\mu)(1-\rho)}C(x,0)$ involves the Riemann-Liouville fractional integral operator of order $(1-\mu)(1-\rho)$ evaluated in the limit as $t \to 0$. C(x,t) is the concentration of solute and f(x) is the real valued function. The solution of (14), subject to the given conditions is

$$C(x,t) = \frac{t^{\mu+\rho(1-\mu)-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\ \mu+\rho(1-\mu)} [(ivk + \mathcal{D}k^2)t^{\mu}] e^{-ikx} f^*(k) \, dk,$$

where $E_{\alpha,\beta}(.)$ is the two parameter Mittag-Leffler function.

2. When $\rho = 1$, Hilfer derivative reduces to the Caputo fractional derivative operator, and Theorem 4.1 reduces to

THEOREM 5.2. Consider the time fractional advection dispersion equation

$${}^{C}D_{0}^{\mu}C(x,t) = -v \frac{\partial C(x,t)}{\partial x} + \mathcal{D} \frac{\partial^{2}C(x,t)}{\partial x^{2}} - \lambda C(x,t), \quad x \in (-\infty,\infty), \ t > 0 \quad (15)$$

with initial and boundary conditions

0.

$$C(x,0)=f(x), \quad 0<\mu<1, \quad \lim_{x\to\infty}C(x,t)=$$

where ${}^{C}D_{0}^{\mu}$ is the Caputo derivative. C(x,t) is the concentration of solute and f(x) is the real valued function. Solution of (15), subject to the given conditions is

$$C(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} E_{\mu} [(-\lambda + ivk + \mathcal{D}k^2)t^{\mu}] e^{-ikx} f^*(k) dk,$$

where $E_{\mu}(.)$ is one parameter Mittag-Leffler function.

3. When $\rho = 0$, Hilfer derivative becomes the Riemann-Liouville fractional derivative operator, defined by equation (4). Theorem 4.1 reduces to

THEOREM 5.3. Consider the time fractional advection dispersion equation

$${}^{RL}D_0^{\mu}C(x,t) = -v \frac{\partial C(x,t)}{\partial x} + \mathcal{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \lambda C(x,t), \quad x \in (-\infty,\infty), \ t > 0$$
(16)

with initial and boundary conditions

$${}^{RL}D_0^{1-\mu}C(x,0) = f(x), \quad 0 < \mu < 1, \qquad \lim_{|x| \to \infty} C(x,t) = 0, \quad t > 0,$$

where ${}^{RL}D_0^{\mu}$ is the Riemann-Liouville derivative. C(x,t) is the concentration of solute and f(x) is the real valued function. Solution of (16), subject to the given conditions is

$$C(x,t) = \frac{t^{\mu-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\mu} [(-\lambda + ivk + \mathcal{D}k^2)t^{\mu}] e^{-ikx} f^*(k) \, dk.$$
(17)

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If we take $\lambda = 0$, equation (17) reduces to the problem discussed by Povstenko et al. [14].

6. Applications

We now discuss an applications of our main Theorem 4.1 for the functions $f(x) = \delta(x)$, the Dirac-delta function, and the exponential function $f(x) = e^{-x}$.

COROLLARY 6.1. Consider time fractional advection dispersion equation

$$D_0^{\mu,\rho}C(x,t) = -v \frac{\partial C(x,t)}{\partial x} + \mathcal{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \lambda C(x,t), \quad x \in (-\infty,\infty), \ t > 0$$

with initial and boundary conditions

$$I_0^{(1-\mu)(1-\rho)}C(x,0) = \delta(x), \quad 0 < \mu \le 1, \ 0 \le \rho \le 1, \quad \lim_{|x| \to \infty} C(x,t) = 0, \quad t > 0.$$

where $\delta(x)$ is Dirac-Delta function. The concentration C(x,t) is given by

$$C(x,t) = \frac{t^{\mu+\rho(1-\mu)-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\ \mu+\rho(1-\mu)} [(-\lambda+ivk+\mathcal{D}k^2)t^{\mu}] e^{-ikx} \, dk.$$

COROLLARY 6.2. Consider time fractional advection dispersion equation

$$D_0^{\mu,\rho}C(x,t) = -v \frac{\partial C(x,t)}{\partial x} + \mathcal{D} \frac{\partial^2 C(x,t)}{\partial x^2} - \lambda C(x,t), \quad x \in (-\infty,\infty), \ t > 0$$

with initial and boundary conditions

$$I_0^{(1-\mu)(1-\rho)}C(x,0) = e^{-x}, \quad 0 < \mu \le 1, \ 0 \le \rho \le 1, \qquad \lim_{|x| \to \infty} C(x,t) = 0, \quad t > 0.$$

Then the solute concentration C(x,t) is given by

$$C(x,t) = \frac{t^{\mu+\rho(1-\mu)-1}}{2\pi} \int_{-\infty}^{\infty} E_{\mu,\ \mu+\rho(1-\mu)} [(-\lambda+ivk+\mathcal{D}k^2)t^{\mu}] e^{-ikx} g(k) \, dk,$$

where $g(k) = \frac{1}{2\pi} \left[\frac{e^{-(1+ik)}-1}{1+ik} \right].$

If we take $\rho = 0$, $\mu = 1$ and $\lambda = 0$, Corollary 6.1 reduces to the result discussed by Pandey et al. [12].

7. Illustration And Discussion

To obtain the effect of fractional order derivatives to the advection dispersion equation with decay term, we compare the analytic solution obtained with the experimental data. Figures are simulations of the concentration of chloride as a function of time and the distance from a point or line source in an aquifer with known properties and are plotted in Matlab with hydraulic conductivity = $2.5 \times 10^{-5} m/s$; hydraulic gradient = 0.001; effective porosity = 0.25; effective diffusion coefficient = $0.75 \times 10^{-9} m^2/s$,

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 $\lambda = 1.32 \text{ days}^{-1}$, $v = 1 \times 10^{-7} m/s$, $\mathcal{D} = 1.9 \times 10^{-7} m^2/s$. The aquifer properties for reference purpose have been taken from [19, p. 384]. Graphs are plotted for fractional and integer order values of μ and ρ in the advection dispersion equation (7) for x = 0, $f(x) = \delta(x)$, the Dirac delta function.

Solution of fractional advection dispersion equation is plotted graphically for Riemann-Liouville case ($\rho = 0$) in Figure 2 and for Caputo derivative case ($\rho = 1$) in Figure 3 for the values $\mu = 1$, 0.95, 0.90, $\rho = 1$, respectively. The solution of fractional advection dispersion equation (7) is plotted graphically for values $\rho = 0.90$ and $\mu = 1$, 0.95, 0.90, respectively in Figure 4.



Figure 2: Concentration profile of chloride varying with time for $\rho = 0$ i.e. the derivative involved is Riemann Liouville fractional derivative



Figure 3: Concentration profile of chloride varying with time for $\rho = 1$ i.e. the derivative involved is Caputo fractional derivative.

The Caputo fractional derivative is more appropriate in solving the real-world problems compared to the Riemann-Liouville fractional derivative because it allows

traditional initial and boundary conditions to be included in the formulation of the problem as already mentioned in Remark 3.1.



Figure 4: Concentration profile of chloride varying with time for $\rho = 0.90$.

Development of the advection dispersion equation begins with assumptions about the random behavior of a single particle, possible velocities in a flow field and the length of time it may hold. Fractional advection dispersion equation can arise, with a non integer-order derivative on time or space variables. Fractional advection dispersion equation are nonlocal i.e. they describe the effect on transport by hydraulic conditions at a distance. Time fractional advection-dispersion equation arise as a result of power law particle residence time distributions and describe particle motion with memory in time. The numerical simulation in Figures 2, 3 and 4 shows that the order of derivative plays an important role on the concentration profile of the pollutant.

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