Super-diffusive Transport Processes in Porous Media

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Abstract The basic assumption of models for the transport of contaminants through soil is that the movements of solute particles are characterized by the Brownian motion. However, the complexity of pore space in natural porous media makes the hypothesis of Brownian motion far too restrictive in some situations. Therefore, alternative models have been proposed. One of the models, many times encountered in hydrology, is based in fractional differential equations, which is a one dimensional fractional advection diffusion equation where the usual second-order derivative gives place to a fractional derivative of order α, with $1 < \alpha \leq 2$. When a fractional derivative replaces the second order derivative in a diffusion or dispersion model, it leads to anomalous diffusion, also called super-diffusion. We derive analytical solutions for the fractional advection diffusion equation with different initial and boundary conditions. Additionally, we analyze how the fractional parameter α affects the behavior of the solutions.

1 Fractional advection diffusion equation

An equation commonly used to describe solute transport is the classical advection diffusion (or dispersion) equation

$$\frac{\partial u}{\partial t}(x,t) = -V\frac{\partial u}{\partial x}(x,t) + D\frac{\partial^2 u}{\partial x^2}(x,t), \tag{1}$$

where u is the concentration, V the average linear velocity, x is the spatial domain, t is the time and $D > 0$ is a constant diffusion (or dispersion) coefficient. The classical advection diffusion equation uses second-order Fickian diffusion which is based on the assumption that solute particles undergo an addition of successive increments

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that are independent, where identically distributed random variables have finite variance and the distribution of the sum of such increments is a normal distribution. Therefore, the fundamental solutions of the classical advection diffusion equation will be Gaussian densities with means and variations based on the values of the coefficients V and D.

The anomalous diffusion extends the capabilities of models built on the stochastic process of Brownian motion. For instance, the movement of particles may not follow Brownian motion because high velocity regions in soil tend to be spatially continuous at all scales. A particle traveling faster or slower than the mean is much more likely to do so over a large distance and it seems to have a spatial memory, a feature that is absent in Brownian motion. Motions with the persistence in movements can be simulated with Lévy motion which assumes that significant deviations from the mean can occur, where large jumps are more frequent than in the Brownian motion. When describing scale dependent transport in porous media, Lévy motion can be seen as a generalization of Brownian motion.

Fractional diffusion was firstly proposed by Chaves [3]. He presents an advection diffusion equation able to generate the Lévy distribution, with the purpose of having a model suitable to investigate the mechanism of super-diffusion. The classical advection diffusion equation (1) can be seen as the combination of the continuity equation

$$\nabla \cdot \mathbf{j} + \frac{\partial u}{\partial t} = 0, \tag{2}$$

with the Fick's empirical law

$$\mathbf{j} = -D\frac{\partial u}{\partial x} + Vu. \tag{3}$$

Chaves [3] proposes to generalize Fick's law to the form

$$\mathbf{j} = -\frac{D}{2}\left(\frac{\partial^{\alpha-1}u}{\partial x^{\alpha-1}} + \frac{\partial^{\alpha-1}u}{\partial(-x)^{\alpha-1}}\right) + Vu, \tag{4}$$

where u is the resident solute concentration, V is the average pore-water velocity, x is the spatial coordinate, t is the time, D is the diffusion coefficient, α is the order of the fractional differentiation and $1 < \alpha \leq 2$. The fractional advection diffusion equation was later generalized by Benson *et al.* [1, 2], to include a parameter β, given by

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = D\left(\frac{1}{2} + \frac{\beta}{2}\right)\frac{\partial^{\alpha}u}{\partial x^{\alpha}} + D\left(\frac{1}{2} - \frac{\beta}{2}\right)\frac{\partial^{\alpha}u}{\partial(-x)^{\alpha}}, \tag{5}$$

where β is the relative weight of solute particle forward versus backward transition probability. For $-1 \leq \beta \leq 0$, the transition probability is skewed backward, while for $0 \leq \beta \leq 1$ the transition probability is skewed forward. For $\beta = 0$, we obtain the model presented in [3], that is, the transition of the solute particles is symmetric.

If we define the fractional operator by

$$2\nabla^{\alpha}_{\beta} = (1+\beta)\frac{\partial^{\alpha} u}{\partial x^{\alpha}} + (1-\beta)\frac{\partial^{\alpha} u}{\partial(-x)^{\alpha}},$$

the equation can be defined in a simple form

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = D\nabla^{\alpha}_{\beta} u. \tag{6}$$

Let us now define the fractional derivatives. The Riemann-Liouville fractional derivatives of order α of a function $u(x,t)$, for $x \in [a,b]$, $-\infty \le a < b \le \infty$, are in general defined by

$$\frac{\partial^{\alpha} u}{\partial x^{\alpha}}(x,t) = \frac{1}{\Gamma(n-\alpha)}\frac{\partial^{n}}{\partial x^{n}}\int_{a}^{x}\frac{u(\xi,t)}{(x-\xi)^{\alpha-n+1}}d\xi,\ n=[\alpha]+1,\ x>a, \tag{7}$$

$$\frac{\partial^{\alpha} u}{\partial(-x)^{\alpha}}(x,t) = \frac{(-1)^{n}}{\Gamma(n-\alpha)}\frac{\partial^{n}}{\partial x^{n}}\int_{x}^{b}\frac{u(\xi,t)}{(\xi-x)^{\alpha-n+1}}d\xi,\ n=[\alpha]+1,\ x<b, \tag{8}$$

where $\Gamma(\cdot)$ is the Gamma function. Therefore in our case, for $1 < \alpha \le 2$ we have

$$\frac{\partial^{\alpha} u}{\partial x^{\alpha}}(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^{2}}{\partial x^{2}}\int_{a}^{x}\frac{u(\xi,t)}{(x-\xi)^{\alpha-1}}d\xi \quad x>a, \tag{9}$$

$$\frac{\partial^{\alpha} u}{\partial(-x)^{\alpha}}(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^{2}}{\partial x^{2}}\int_{x}^{b}\frac{u(\xi,t)}{(\xi-x)^{\alpha-1}}d\xi, \quad x<b. \tag{10}$$

There are a number of interesting books describing the analytical properties of fractional derivatives, such as, [5, 8, 13, 14, 16, 17].

2 Exact Solutions

In this section we show how to obtain exact solutions for some problems involving the fractional advection diffusion equation. The first problem is related to models that appear in works such as, Benson *et al.* [2], Huang *et al.* [6], Pachepsky *et al.* [15], Zhou *et al.* [24]. The second problem considers the Dirac delta function as the initial condition, which is of interest in many applications. Although we consider exact solutions, numerical solutions have also being investigated for super-diffusive models represented by equation (5) and for some values of β, namely finite element methods [4, 7, 19, 22], finite volume methods [23], spectral methods [10] and finite difference methods [11, 20, 21].

Let us now consider the problem which consists of equation (5) defined in the whole real line, $x \in \mathbb{R}$, and $t > 0$, with the initial condition

$$u(x,0) = \begin{cases} u_0, & x<0 \\ m_0, & x=0 \\ 0, & x>0, \end{cases} \tag{11}$$

where u_0 and m_0 are constants. The boundary conditions are given by

$$\lim_{x\to-\infty} u(x,t) = u_0, \qquad \lim_{x\to\infty} u(x,t) = 0. \tag{12}$$

We derive the exact solution for this problem by using the Fourier transform. If we consider a function defined in $\mathbb{R}$, then we can define its Fourier transform which is given by

$$\mathscr{F}[f(x)] = \hat{f}(k) = \int_{-\infty}^{+\infty} f(\tau)\mathrm{e}^{ik\tau}d\tau,$$

and its inverse is given by

$$f(x) = \mathscr{F}^{-1}[\hat{f}(k)] = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \hat{f}(\xi)\mathrm{e}^{-ix\xi}d\xi.$$

The well-known Fourier transforms for integer derivatives are given by

$$\mathscr{F}\left[\frac{\partial^n f}{\partial x^n}\right] = (-ik)^n f(k).$$

They can be extended to rational order such as

$$\mathscr{F}\left[\frac{\partial^\alpha f}{\partial x^\alpha}\right] = (-ik)^\alpha \hat{f}(k), \qquad \mathscr{F}\left[\frac{\partial^\alpha f}{\partial (-x)^\alpha}\right] = (ik)^\alpha \hat{f}(k).$$

In the next proposition we state the solution for the problem (5), (11), (12).

Proposition 1: The exact solution for the fractional advection diffusion equation (5), where $1 < \alpha \leq 2$ and $-1 \leq \beta \leq 1$, subject to the initial condition (11) and with boundary conditions (12), is of the form

$$u(x,t) = u_0\left[1 - F_{\alpha\beta}\left(\frac{x - Vt}{(RDt)^{1/\alpha}}\right)\right], \tag{13}$$

where $F_{\alpha\beta}$ is the cumulative probability function and $R = |\cos(\frac{\pi\alpha}{2})|$. For $\alpha \neq 1$ and $x \geq 0$ the cumulative probability function is defined by

$$F_{\alpha\beta}(x) = 1 - \frac{1}{2}\int_{-\theta}^{1} \exp\left[-(cx)^{\alpha/(\alpha-1)}U_\alpha(\phi,\theta)\right]d\phi, \tag{14}$$

where

$$c = \left[1 + \left(\beta\tan\frac{\pi\alpha}{2}\right)^2\right]^{-1/2\alpha},$$

$$\theta = \frac{2}{\pi\alpha}\tan^{-1}\left[\beta\tan\frac{\pi\alpha}{2}\right],$$

$$U_\alpha(\phi,\theta)=\left[\frac{\sin(\pi\alpha(\phi+\theta)/2)}{\cos(\pi\phi/2)}\right]^{\frac{\alpha}{1-\alpha}}\frac{\cos(\pi(\alpha-1)\phi/2+\alpha\theta)}{\cos(\pi\phi/2)}.$$

The function $F_{\alpha\beta}(x)$ for $\alpha\neq 0$ and $x<0$ is computed using the identity

$$F_{\alpha\beta}(-x)=1-F_{\alpha,-\beta}(x)$$

and $F_{\alpha\beta}(-\infty)=0,\quad F_{\alpha\beta}(\infty)=1.$

Note that in order to have $u(x,t)\to u(x^0,0)$ as $(x,t)\to(x^0,0)$, for each $x^0\in\mathbb{R}$, the constant m_0, in the initial condition (11), is defined as

$$m_0=\frac{u_0}{2}(1+\theta).$$

Proof: Applying the Fourier transform at (5) we obtain

$$\frac{d}{dt}\hat{u}(k,t)=ikV\hat{u}(k,t)+\frac{1}{2}(1+\beta)D(-ik)^\alpha\hat{u}(k,t)+\frac{1}{2}(1-\beta)D(ik)^\alpha\hat{u}(k,t).\quad(15)$$

This is an ordinary differential equation which solution is given by

$$\hat{u}(k,t)=A\exp\left(\frac{1}{2}(1+\beta)(-ik)^\alpha Dt+\frac{1}{2}(1-\beta)(ik)^\alpha Dt+ikVt\right),\quad(16)$$

and the constant A is determined using the initial condition, that is, $A=\hat{u}(k,0)$. We have

$$\hat{u}(k,t)=\hat{u}(k,0)\exp\left(\frac{1}{2}|k|^\alpha Dt\left(\cos\left(\alpha\frac{\pi}{2}\right)-i\beta\sin\left(\text{sign}(k)\alpha\frac{\pi}{2}\right)\right)+ikVt\right).$$

After some algebra this can be written as

$$\hat{u}(k,t)=\hat{u}(k,0)\exp\left(\cos(\pi\alpha/2)Dt|k|^\alpha(1-i\beta(sign(k))\tan(\pi\alpha/2))+ikVt\right).\quad(17)$$

Therefore, noticing that $\cos(\alpha\pi/2)$ is negative for $1<\alpha\leq 2$, we have

$$\hat{u}(k,t)=\hat{u}(k,0)\psi_\beta(k),\quad(18)$$

where

$$\psi_\beta(k)=\exp\left(-|\cos(\pi\alpha/2)|Dt|k|^\alpha(1-i\beta(sign(k))\tan(\pi\alpha/2))+ikVt\right).$$

We note $\psi_\beta(k)$ is a characteristic function. The cumulative probability function determined by the characteristic function and the densities, which are the differentiation of the cumulative probability, will be denoted by $F_{\alpha,\beta}$ and $f_{\alpha,\beta}$ respectively. According to McCulloh et al [9] (pag. 308, equation (3)), for the characteristic function $\psi_\beta(k)$ we obtain

$$\mathscr{F}^{-1}[\psi_\beta(k)]=f_{\alpha\beta}(x,\sigma,\delta),$$

and

$$F'_{\alpha\beta}(x,\sigma,\delta) = f_{\alpha\beta}(x,\sigma,\delta),$$

for

$$\delta = Vt \quad , \quad \sigma = (RDt)^{1/\alpha} \quad \text{and} \quad R = |\cos(\pi\alpha/2)|.$$

Note that

$$F'_{\alpha\beta}(x,\sigma,\delta) = F_{\alpha\beta}\left(\frac{x-\delta}{\sigma},1,0\right) := F_{\alpha\beta}\left(\frac{x-\delta}{\sigma}\right),$$

where $F_{\alpha\beta}$ is defined by (14). Consequently, using the convolution property for Fourier transforms the inversion of (18) is given by

$$u(x,t) = \int_{-\infty}^{\infty} u(\tau,0) f_{\alpha\beta}(x-\tau,\sigma,\delta)d\tau.$$

Since $u(x,0) = 0$ for $x > 0$ and $u(x,0) = u_0$ for $x < 0$ we have

$$u(x,t) = \int_{-\infty}^{0} u_0 f_{\alpha\beta}(x-\tau,\sigma,\delta)d\tau.$$

Changing variables, by considering $\xi = x - \tau$, we have

$$u(x,t) = u_0 \int_{x}^{\infty} f_{\alpha\beta}(\xi,\sigma,\delta)d\xi.$$

Therefore

$$\begin{aligned} u(x,t) &= u_0[\lim_{\xi\to\infty} F_{\alpha\beta}(\xi,\sigma,\delta) - F_{\alpha\beta}(x,\sigma,\delta)] \\ &= u_0[1 - F_{\alpha\beta}(x,\sigma,\delta)] := u_0\left[1 - F_{\alpha\beta}\left(\frac{x-Vt}{(RDt)^{1/\alpha}}\right)\right]. \end{aligned}$$

Finally

$$u(x,t) = u_0\left[1 - F_{\alpha\beta}\left(\frac{x-Vt}{(RDt)^{1/\alpha}}\right)\right]. \tag{19}$$

□

Let us now consider the problem when the transition of the solute particle is symmetric, that is, $\beta = 0$. The problem is defined in the whole line, $x \in \mathbb{R}$, and $t > 0$, with initial conditions (11) and boundary conditions (12). This example was considered in [20].

Corollary 2: The exact solution for the fractional advection diffusion equation (5), with $\beta = 0$, subject to the initial condition (11) and with boundary conditions (12) is of the form

$$u(x,t) = u_0\left[1 - F_{\alpha}\left(\frac{x-Vt}{(RDt)^{1/\alpha}}\right)\right], \tag{20}$$

where F_α is the cumulative probability function and $R = |\cos(\frac{\pi\alpha}{2})|$. For $\alpha \neq 1$ and $x \geq 0$ the cumulative probability function is defined by

$$F_\alpha(x) = 1 - \frac{1}{2}\int_0^1 \exp\left[-x^{\alpha/(\alpha-1)} U_\alpha(\phi)\right] d\phi, \tag{21}$$

where

$$U_\alpha(\phi) = \left[\frac{\sin(\pi\alpha\phi/2)}{\cos(\pi\phi/2)}\right]^{\frac{\alpha}{1-\alpha}} \frac{\cos(\pi(\alpha-1)\phi/2)}{\cos(\pi\phi/2)}.$$

The function $F_\alpha(x)$ for $\alpha \neq 0$ and $x < 0$ is computed using the identity

$$F_\alpha(-x) = 1 - F_\alpha(x)$$

and $F_\alpha(-\infty) = 0, \quad F_\alpha(\infty) = 1.$

Note that in order to have $u(x,t) \to u(x^0, 0)$ as $(x,t) \to (x^0, 0)$, for each $x^0 \in \mathbb{R}$, the constant m_0, in the initial condition (11), is defined as

$$m_0 = \frac{u_0}{2}.$$

Consider now the definition of a α-stable error function, Serf_α

$$\mathrm{Serf}_\alpha(z) = 2\int_0^z f_\alpha(x)dx,$$

where $f_\alpha(x) := F_\alpha^{'}(x)$. Note that

$$\mathrm{Serf}_\alpha(z) = 2\int_0^z f_\alpha(x)dx = 2\left(\int_{-\infty}^z f_\alpha(x)dx - \frac{1}{2}\right).$$

Therefore we can also write the solution (20) in the form

$$u(x,t) = \frac{u_0}{2}\left[1 - \mathrm{Serf}_\alpha\left(\frac{x - Vt}{(RDt)^{1/\alpha}}\right)\right]$$

For $\alpha = 2$, we have

$$u(x,t) = \frac{u_0}{2}\left[1 - \mathrm{Erf}\left(\frac{x - Vt}{2\sqrt{Dt}}\right)\right]$$

where Erf is the error function. Note that in this case we have the usual advection diffusion equation with the second order derivative.

A similar solution is the named Ogata and Banks solution [12]

$$u(x,t) = \frac{u_0}{2}\left[1 - \mathrm{Erf}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + e^{Vx/D}\mathrm{Erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$

where Erfc is the complementary error function. However, this is a solution of a slightly different problem. This is a solution for a problem defined in the half-line, that is, $x \geq 0$, with initial condition

$$u(x,0) = 0, \tag{22}$$

and boundary conditions

$$u(0,t) = u_0, \qquad u(\infty,t) = 0. \tag{23}$$

We note that for very small diffusion the solutions are basically the same. Nevertheless, if we want to consider such initial and boundary conditions, (22) and (23), with the fractional advection diffusion equation we need to derive a different exact solution and we cannot use Fourier transforms.

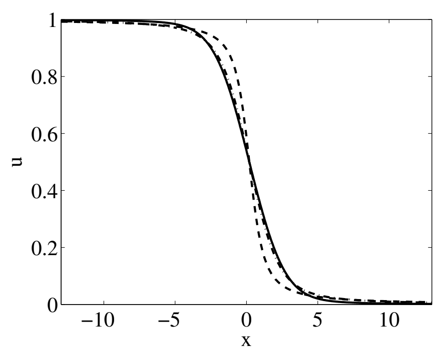

Fig. 1 Solutions for problem (5), (11), (12) for $t = 2$ with $V = 0.1$, $D = 1$, $\beta = 0$ and for different values of α: $\alpha = 1.8$ (−), $\alpha = 1.5$ (− · −), $\alpha = 1.2$ (−−).

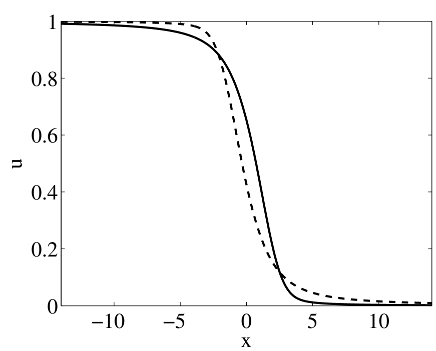

Fig. 2 Solutions for problem (5), (11), (12) for $t = 2$ with $V = 0.1$, $D = 1$, $\alpha = 1.5$ and for different values of β: $\beta = 0.6$ (−−), $\beta = -0.6$ (−).

In Fig.1 and Fig. 2 we plot the effect of the fractional order α and the effect of the skewness parameter β on the solution of the problem. To compute the integrals in (13) we have used Gauss-Legendre quadrature. In Fig. 1 we observe how the α

affects the solution for a fixed β, namely $\beta = 0$. As α gets larger we see the diffusive effects increase. In Fig. 2 we show how the β affects the solution, for a fixed α. The solution moves backward or forward according to the sign of the parameter β.

Next, we present the solution of the problem that considers the fractional advection diffusion equation with the Dirac delta function as the initial condition, that is,

$$u(x,0) = \delta(x), \tag{24}$$

and subject to the boundary conditions,

$$\lim_{x\to-\infty} u(x,t) = 0, \qquad \lim_{x\to\infty} u(x,t) = 0. \tag{25}$$

Similarly to what we have done previously, we use Fourier transforms to derive the exact solution.

Proposition 3: The exact solution for the problem (5), (24), (25) is given by

$$u(x,t) = \frac{1}{2\pi}\int_0^\infty e^{(1/2)\xi^\alpha Dt\cos(\alpha\pi/2)}\cos(\beta\xi^\alpha DT\sin(\alpha\pi/2)+\xi(x-Vt))d\xi. \tag{26}$$

Proof: Following the same steps as in the previou proposition and knowing that $\hat{u}(k,0) = \hat{\delta}(k) = 1$, we have

$$\hat{u}(k,t) = \exp\left(\frac{1}{2}(1+\beta)(-ik)^\alpha Dt + \frac{1}{2}(1-\beta)(ik)^\alpha Dt + ikVt\right). \tag{27}$$

After some algebra this can be written as

$$\hat{u}(k,t) = \exp\left(\frac{1}{2}|k|^\alpha Dt\left(\cos\left(\alpha\frac{\pi}{2}\right) - i\beta\sin\left(\mathrm{sign}(k)\alpha\frac{\pi}{2}\right)\right) + ikVt\right). \tag{28}$$

By the Fourier inversion

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^\infty e^{(1/2)\xi^\alpha Dtg(\xi,\alpha,\beta)}e^{-i\xi(x-Vt)}d\xi,$$

where $g(\xi,\alpha,\beta) = \cos(\alpha\pi/2) - i\beta\sin(sign(\xi\alpha\pi/2))$. Then

$$u(x,t) = \frac{1}{2\pi}\left[\int_0^\infty e^{(1/2)\xi^\alpha Dtg(-\xi,\alpha,\beta)}e^{i\xi(x-Vt)}d\xi + \int_0^\infty e^{(1/2)\xi^\alpha Dtg(\xi,\alpha,\beta)}e^{-i\xi(x-Vt)}d\xi\right].$$

After some calculations we get the result (26). □

For the particular case, when $\beta = 0$, where the transition probability is symmetric, we have the following result.

Corollary 4: The exact solution for the problem (5), (24), (25), with $\beta = 0$, is given by

$$u(x,t) = \frac{1}{2\pi}\int_0^\infty \mathrm{e}^{(1/2)\xi^\alpha Dt\cos(\alpha\pi/2)}\cos(\xi(x-Vt))d\xi. \qquad (29)$$

In Fig. 3 and Fig. 4 we represent the behavior of the exact solution for the problem (5), (24), (25). Again the integral in (26) has been computed with Gauss-Legendre quadrature. In Fig. 3 we observe the effect of α for a fixed β. For larger values of α we have a more diffusive behavior. However, the shape of the function does not change too much appart from the expected damping. In Fig. 4 we display the effect of changing β assuming a fixed α. We observe the shape changes forming long tails on the left or right according to the sign of β.

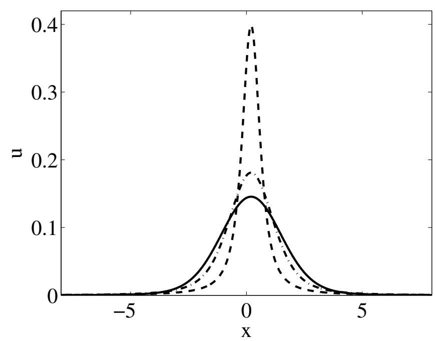

Fig. 3 Solutions for the problem (5), (24), (25) for $t = 2$ with $V = 0.1$, $D = 1$, $\beta = 0$ for different values of α: $\alpha = 1.8$ (−), $\alpha = 1.5$ (− · −), $\alpha = 1.2$ (−−).

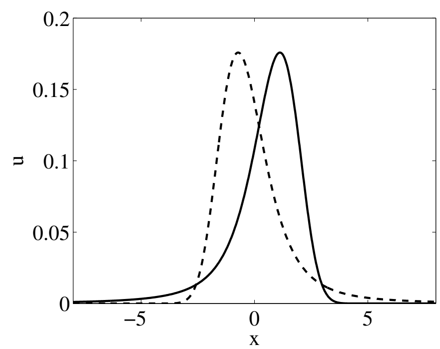

Fig. 4 Solutions for the problem (5), (24), (25) for $t = 2$ with $V = 0.1$, $D = 1$, $\alpha = 1.5$ for different values of β: $\beta = 0.5$ (−−), $\beta = -0.5$ (−).

3 Final Remarks

We have presented a fractional advection diffusion equation subject to different initial conditions and boundary conditions and have shown how we can obtain exact solutions by using Fourier transforms. We have also observed how the parameters α and β affects the shape of the solution. This model is more suitable to describe certain real world problems than the classical advection diffusion equation as shown in many examples in literature. When adjusting the model to some physical problem, additionally to the estimation of the parameters V and D, we can also estimate the parameters α and β to obtain the model that more successfully describe our physical situation.

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