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The fractional-order governing equation of Lévy motion

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Abstract. A governing equation of stable random walks is developed in one dimension. This Fokker-Planck equation is similar to, and contains as a subset, the second-order advection dispersion equation (ADE) except that the order (α) of the highest derivative is fractional (e.g., the 1.65th derivative). Fundamental solutions are Lévy's α-stable densities that resemble the Gaussian except that they spread proportional to time$^{1/\alpha}$, have heavier tails, and incorporate any degree of skewness. The measured variance of a plume undergoing Lévy motion would grow faster than Fickian plume, at a rate of time$^{2/\alpha}$, where $0 < \alpha \leq 2$. The equation is parsimonious since the parameters are not functions of time or distance. The scaling behavior of plumes that undergo Lévy motion is accounted for by the fractional derivatives, which are appropriate measures of fractal functions. In real space the fractional derivatives are integrodifferential operators, so the fractional ADE describes a spatially nonlocal process that is ergodic and has analytic solutions for all time and space.

1. Introduction

Solutes that move through aquifers do not generally follow a Fickian, second-order, governing equation because of large deviations from the stochastic process of Brownian motion. The most common methods to incorporate relatively large particle motions include treating the parameters and dependent variables of the advection dispersion equation (ADE) as random and correlated, leading to a local, scale-dependent effective dispersion tensor [*Gelhar and Axness*, 1983; *Dagan*, 1984, 1988; *Neuman and Zhang*, 1990]. This local approach is handy because analytic solutions are available; however, it assumes that a Gaussian model is reasonably appropriate at all scales. In developing these equations, a Fickian model is typically assumed at some small scale. Nonlocal methods [e.g., *Neuman*, 1993; *Deng et al*., 1993; *Cushman et al*., 1994] can model long-range spatial and/or temporal correlation of particle and can do away with the Fickian assumption. The nonlocal forms are typically solved in Fourier/Laplace space [e.g., *Deng et al*., 1993]. The most general formulations [*Cushman et al*., 1994] allow virtually any space-time structure to solute movement, although measurement of the Fourier/Laplace dispersion tensor is not straightforward. All theories that develop a local dispersion coefficient, and some of the nonlocal methods, are based on finite velocity autocorrelation models. *Molz et al*. [1997], *Liu and Molz* [1997a, b], and *Painter* [1996a, b, 1997] have called this most basic assumption about aquifer properties into question. This study looks at the governing equation of motions with finite or infinite variance from a Fokker-Planck perspective. The classical, deterministic ADE is a subset of this equation, just as Brownian motion is a subset of Lévy motion. The governing equation uses fractional derivatives, which are appropriate measuring tools to use on fractal functions [*Kolwankar and Gangal*, 1996; *Stiassnie*, 1997]. The simplest form of this equation, shown herein, retains a spatially nonlocal form but describes an ergodic Markov process at all times.

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Solute transport in subsurface material may be viewed as a purely probabilistic problem [e.g., *Cushman*, 1990; *Bhattacharya and Gupta*, 1990]. This approach is intimately tied to the classical divergence (Eulerian) point of view through a string of mathematical equivalences. *Einstein* [1956] first explored this method by assuming that a single microscopic particle was continuously bombarded by other particles, resulting in Brownian random walk. By assuming a finite variance process and taking appropriate limits, he found that the resulting Green's function of the probability of finding a particle somewhere in space was a Gaussian (Normal) probability density. If the motions of a large number of particles are assumed independent, then the particle probability and the concentration of a diffusing tracer are interchangeable, leading to the equivalence of the process of Brownian motion and the governing equation $\partial C/\partial t = \mathcal{D}\nabla^2 C$. The most important assumption tied to Brownian motion and the second-order, Fickian diffusion equation is that a particle's motion has little or no spatial correlation. Since long walks in the same direction are rare, the variance of a particle's excursion distance is finite.

The classical descriptions of a local dispersion tensor based on the second-order diffusion equation [*Gelhar and Axness*, 1983; *Dagan*, 1984, 1988; *Neumann and Zhang*, 1990] carry similar assumptions: The aquifer velocity contrasts must be small and the mean travel distance must be large compared to a typical velocity correlation length. These assumptions arise

because the dispersion part of the ADE is essentially a restatement of DeMoive's central limit theorem: a large number of finite variance particle trajectories (random variables) must be added before a Gaussian appears. Tracer particles released into aquifers experience large velocity contrasts along their trajectories. Recent theories devised to explain non-Fickian dispersion in turbulent and chaotic systems [e.g., *Shlesinger et al*., 1982; *Klafter et al*., 1987; *Zaslavsky*, 1994a; *Saichev and Zaslavsky*, 1997] begin with the assumption that particle excursion distances and velocities are likely to have large, even infinite, variance. Since the trajectories are (or belong to the domain of attraction of) stable variables, these transitions converge relatively quickly to a non-Gaussian limit distribution. The result is that a tracer test need not sample large volumes before it can be described by a single, self-contained equation, if the motions are well modeled by an infinite variance (e.g., power law) model. However, the second-order ADE is not the governing equation of these movements.

Physicists, chemists, engineers, economists, and hydrologists are using infinite variance models to conveniently describe realistic processes that are dominated by extreme events [e.g., *Mandelbrot*, 1963; *Fama*, 1965; *Shlesinger et al*., 1982, 1987, 1995; *Nikias and Shao*, 1995; *Anderson and Meershaert*, 1998; *Adler et al*., 1998]. Motivated by diffusion in fractals [*Giona and Roman*, 1992], motion in chaotic [*Zaslavsky*, 1994a, b] and turbulent flow [*Shlesinger et al*., 1987], Fokker-Planck equations have been developed that use fractional derivatives. These derivatives are nonlocal operators that incorporate spatial and/or temporal memory. In particular, a spatial fractional derivative describes particles that move with long-range spatial dependence or high velocity variability [*Benson*, 1998; *Benson et al*., 2000]. These motions fall within a very general model of particle motion called continuous time random walks (CTRW) [*Montroll and Weiss*, 1965; *Scher and Lax*, 1973]. Reviews of CTRW in a hydrologic context are given by *Berkowitz and Scher* [1995] and *Benson* [1998]. The CTRW allow descriptions of particle motions that have extremely long-range temporal and/or spatial correlation. In general, the CTRW eventually converge to Brownian motion unless some infinite moments of the particle excursion time and/or variance are assumed. In these cases, the CTRW converge to motions described by the fractional-order Fokker-Planck equations.

In this study, we review *Benson*'s [1998] derivation of a Fokker-Planck equation for Markovian particle transport, which follows the methodology of *Zaslavsky* [1994a, b]. The choice of Markovian transport results in a greatly simplified derivation. Inherent in this assumption is that all dependence can be explicitly accounted for by spatially heavy-tailed particle excursion probabilities, rather than by temporal correlation functions. We show how the classical ADE results from an assumption of the existence of the second moment of the particle transition probability and then generalize the transition density to include particle walks that favor long-range motions and may include skewness.

2. Local Theories

Because of their relative simplicity and widespread use, we review the basis of local theories, which typically make use of the ADE:

$$\frac{\partial C}{\partial t} = \nabla \cdot (-vC + \mathcal{D}\nabla C), \tag{1}$$

where C is solute concentration and $\mathcal{D}$ and v are local dispersion and velocity tensors, respectively. On a multidimensional, macroscopic scale the concentration is a random function, so C refers to the expected concentration. The ADE is based on the classical definition of the divergence of a vector field. The divergence is defined as the ratio of total flux through a closed surface to the volume enclosed by the surface when the volume shrinks toward zero [e.g., *Schey*, 1992]:

$$\operatorname{div} \mathbf{J} \equiv \lim_{V \to 0} \frac{1}{V} \int_S \mathbf{J} \cdot \mathbf{n}\, dS, \tag{2}$$

where $\mathbf{J}$ is a flux vector, V is an arbitrary volume enclosed by surface S, and $\mathbf{n}$ is a unit vector normal to the surface. This is valid only if the flux is indeed a "point" vector quantity relative to the scale of observation, for example, heat flow in homogeneous material. Then the limit exists and the operator reduces to the familiar dot product with the gradient vector $[\partial/\partial x, \partial/\partial y, \partial/\partial z]$. Solute dispersion is a counterexample since it is primarily due to velocity fluctuations that arise only as an observation space grows larger, invalidating the limit. The solute flux is due to the combined effects of mean velocity (advection) and velocity fluctuations (dispersion). The dispersive fluxes for a given volume are typically averaged in some fashion (volumetric, statistical) and approximated by Fick's first law. Since velocity itself is a variable function of space, as a control volume shrinks (as the divergence requires), the Darcy velocity fluctuations and the dispersive flux disappear. Therefore the true divergence of the macroscopic solute flux cannot contain a macroscopic dispersive term.

Because of the limit in (2), the classical Gauss divergence theorem discounts macrodispersion until the dispersive flux can be approximated by a point vector. This requires a separation of scale: The scale of the transport process must be much larger than some finite volume at which the ratio in (2) becomes relatively constant. For these things to happen, the dispersive flux must not increase as a volume passes some largest size. This representative elementary volume (REV) for dispersion is the point at which deviations in the velocity field are negligible.

However, when a plume is in an intermediate stage not many times larger than a finite velocity autocorrelation distance, a de facto definition of divergence is often used to quantify advection and dispersion. The divergence is associated with a nonzero volume and is given by the first derivative of total surface flux to volume (Figure 1) rather than the limit of the derivative at zero volume. The dispersion coefficient does not grow (scale) if the ratio of surface flux to volume is constant over some range of volume (solid lines in Figure 1). An example is a column of uniform glass beads. At the pore scale the ratio is nonconstant, and no single dispersion parameter can be assigned. At some larger scale the ratio of total surface flux to volume is constant over a large range of arbitrary volumes, and the relatively constant first derivative (the de facto divergence) allows the assignment of a dispersion coefficient. Both volume averaging [*Bear*, 1972] and ensemble averaging [e.g., *Gelhar*, 1986; *Dagan*, 1986] theories are based on this concept of separation, or distinction, of scale.

At the field scale, at least two problems occur that make it difficult to rely on the REV concept. First, even if there is a distinct hierarchy, the act of measurement involves a volume integration, which impacts the dispersion coefficient [*Cushman*, 1984]. Second, there is a long-standing and growing body

of evidence that real geologic materials have evolving heterogeneity [e.g. *Winograd and Pearson*, 1976; *Sposito et al*., 1986; *Wheatcraft and Tyler*, 1988; *Rajaram and Gelhar*, 1995; *Di Federico and Neuman*, 1997]. If this is the case, there will be no separation of scale as in Figure 1a, and the growth of dispersive flux follows the dashed lines in Figure 1, which represent continuous scaling of the solute flux over a relatively large range.

Since many analytic solutions already exist to the classical ADE, it has been advantageous to assume that the nonconstant volumetric surface flux can be approximated by a step function (Figure 1), wherein each rise is described by a growing $\mathcal{D}$. The local parameter $\mathcal{D}$ is intimately tied to a specific volume, and the ADE is no longer self-contained with a closed-form solution for all scales. Typical methods used to estimate the scale-dependent $\mathcal{D}$ rely on a small-perturbation (linearized) stochastic ADE [*Gelhar and Axness*, 1983; *Dagan*, 1984, 1988; *Neuman and Zhang*, 1990] that are limited to relatively homogeneous aquifers. More recent methods [*Serrano*, 1995] can handle high variance through iterative expansions. Many theories recognize that in the midst of continuous heterogeneity, a plume will deviate significantly from a Gaussian and that the effective dispersion coefficient is simply a measure of the time rate of change of the ensemble average plume's second moment [e.g., *Rajaram and Gelhar*, 1995]. Popular descriptions of continuous (evolving) heterogeneity include fractional Brownian motion and fractional Gaussian noise [*Rajaram and Gelhar*, 1995; *Neuman*, 1995; *Kemblowsi and Wen*, 1993; *Zhan and Wheatcraft*, 1996; *Di Federico and Neuman*, 1997, 1998; *Molz et al*., 1997], which require cutoffs (often naturally imposed) to ensure convergence of second moment expressions.

An integer-order divergence theorem forces a scaling parameter, since the ratio of flux to volume is scale-dependent. Rather than use a step function approximation of the growth of the dispersive flux with scale, which forces $\mathcal{D}$ to take on increasing values, one might try to describe the evolving dashed curve in Figure 1b. Nonlocal, including convolutional, theories do this by integrating the cumulative effects of dispersion over any lengthscale and/or timescale. A subset of these uses the mathematical tools of fractional calculus, which are nonlocal operators for fractal functions. Fractional derivatives are attractive because they behave very much like traditional, integer-order derivative operators and allow simple equations and solutions. Further, a large class of random motions directly imply fractional-order governing equations [*Meerschaert et al*., 1999].

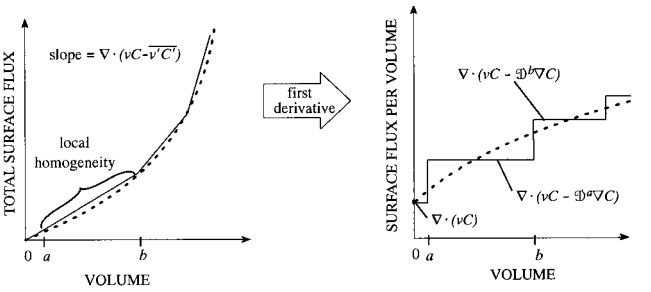

Figure 1. Illustration of the definition of the divergence of solute flux over many scales. Solid lines denote assumption of local homogeneity and multiscale, integer-order (classical) divergence. Dashed lines denote continuum heterogeneity and the resulting noninteger-order divergence. To reconcile the growth in the integer divergence (using local theories) from scale a to b, the first-order fluctuations $\overline{v'C'}$ are approximated by $\mathcal{D}\nabla C$ with increasing, spatially local $\mathcal{D}$.

3. Fokker-Planck Equation

Recently, the governing equation of all stable random walks was developed in multiple dimensions [*Meerschaert et al*., 1999]. Here we derive a simpler one-dimensional (1-D) subset to illustrate the concepts. A Fokker-Planck equation (FPE) describes the change of probability of a random function in space and time, so it is naturally used to describe solute transport. The FPE is a statement about the conservation of probability that a particle will occupy a specific location. At any particular time the sum of the probabilities at all locations must equal unity. So if the probability changes in one location from one moment to the next, the probability must also change in the vicinity to conserve probability. An ensemble of particles (i.e., a large number) can fulfill the probabilities, and the FPE becomes an equation of the conservation of mass.

Derivation of an FPE starts with a simple mathematical statement of how a random measure changes state from one moment to the next after some event has occurred. In this case, we are interested in the probability that a particle has moved from location x_0 to x_2 in the time t_0 to t_2, or $p(x_2 - x_0; t_2 - t_0)$. This probability will be referred to as the transition density, which is conditional on the initial position (x_0) and the time interval. The particle must move through an intermediate location x_1, so this probability can be found by summing over all possible intermediate points x_1. If the process is defined so that a Markov process, in which the movement of a particle is independent of past movements, arises, then the probability of making both transitions (x_0 to x_1 to x_2) is the product of the single-transition probabilities, giving the Chapman-Kolmogorov equation:

$$p(x_2 - x_0; t_2 - t_0) = \int p(x_2 - x_1; t_2 - t_1)p(x_1 - x_0; t_1 - t_0)\, dx_1. \quad (3)$$

The relationship between this transition density and the particle position density (known as the propagator for a single particle) is that the particle position density has moved from (and must incorporate) the initial conditions. The particle's initial position is defined as x_0 at time $t_0 = 0$. Placing this density into (3) and dropping the subscript on x_2 yields

$$p(x - x_0; t) = \int p(x - x_1; t - t_1)p(x_1 - x_0; t_1)\, dx_1. \quad (4)$$

Two different tacks are often used to obtain solutions of the Chapman-Kolmogorov equation. The first uses the fact that convolutions are present and transfers to Fourier/Laplace space for solutions [*Montroll and Weiss*, 1965; *Scher and Lax*, 1973; *Shlesinger et al*., 1982]. The second stays in real space and solves the instantaneous change in probability resulting in a Fokker-Planck differential equation [*Zaslavsky*, 1994a, b]. Similar to equations of conservation of mass, the FPE is a statement of the conservation of probability of a single particle's location over a brief period of time. Since solutions of the FPE are gained via Fourier and Laplace transforms, the two methods are closely related. Staying in real space and realizing that the propagator is the transition from the initial condition to the present time gives a shorthand notation of the density $p(x -$

$x_0; t) = P(x, t)$. Using this shorthand notation, replacing x_1 with ζ and signifying the interval $t - t_1$ by Δt gives a compact form for the next jump:

$$P(x, t + \Delta t) = \int p(x - \zeta; \Delta t) P(\zeta, t)\, d\zeta. \tag{5}$$

To make the next step in the derivation, a requirement on the relative size of the total time (t) versus the transition time (Δt) is sometimes needed. For a general transition density, Δt must be much smaller than the total time, and Δt is called a mixing time. Then an appropriate limit theorem such as the central limit theorem (CLT) can be invoked, implying that a large number of transitions are integrated and a limit distribution is approached. The assumption of a Markovian process requires that all time dependence is contained in this mixing time so that the convolution still holds. If the transitions are independent, identically distributed (iid) stable variables (the standard normal, for example), then no restrictions are placed on the transition time and the convolution is always satisfied. For example, iid Gaussian transitions result immediately in a Gaussian propagator.

By taking infinitesimal values of Δt in (5), we will know the change in $P(x, t)$ over a very short time period, resulting in a differential equation. The limits and moments of the particle transition probability must be correctly identified. One should expect that a particle that travels along fractal paths and/or requires power law times to complete individual walks will have different limiting behavior than a typical Gaussian or finite variance process. We limit this discussion to the first time derivative. An extension to fractional-in-time processes is straightforward [*Zaslavsky*, 1994a, b; *Saichev and Zaslavsky*, 1997; *Benson*, 1998]. The time derivative of p is defined as

$$\frac{\partial p(x - x_0; t)}{\partial t} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} [p(x - x_0; t + \Delta t) - p(x - x_0; t)]. \tag{6}$$

The density $p(x - x_0; t + \Delta t)$ can be replaced by the Markov relation:

$$p(x - x_0; t + \Delta t) = \int p(x - \zeta; \Delta t) p(\zeta - x_0; t - t_0)\, d\zeta. \tag{7}$$

Placing (7) into (6) and recalling the definition $p(x - x_0; t) \equiv P(x, t)$ gives the differential probability change:

$$\frac{\partial P(x, t)}{\partial t} = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left(\int p(x - \zeta; \Delta t) P(\zeta, t)\, d\zeta - P(x, t) \right). \tag{8}$$

The instantaneous transition density has the following limit:

$$\lim_{\Delta t \to 0} p(x - \zeta; \Delta t) = \delta(x - \zeta), \tag{9}$$

where $\delta(x - \zeta)$ is the Dirac delta function, which means that as the transition time tends to zero, the probability that the particle does not move goes to unity. Equivalently, the Fourier transform of the transition density has a limit of unity:

$$\lim_{\Delta t \to 0} \mathcal{F}[(p(x - \zeta; \Delta t)] \equiv \lim_{\Delta t \to 0} \hat{p}(k; \Delta t) = 1, \tag{10}$$

where the circumflex and change of variable from x to k indicates Fourier transform. This density has all positive moments equal to zero. When Δt is nonzero, the density has higher-order moments. The first moment of this instantaneous transition density is defined by the expected value of the particle's new position minus the initial position:

$$A(\Delta t) = \int (x - \zeta) p(x - \zeta; \Delta t)\, dx. \tag{11}$$

The second moment of many power law functions and most of Lévy's α-stable instantaneous transition densities is infinite; therefore we choose a coefficient $B(\Delta t)$ that is a measure of the spread of the density similar to the second moment of a Gaussian. A very general transition density with finite or infinite variance has a Fourier transform:

$$\hat{p}(k; \Delta t) = 1 - A(\Delta t)(ik) + \tfrac{1}{2} B(\Delta t)[(1 + \beta)(ik)^\alpha + (1 - \beta)(-ik)^\alpha] + \mathcal{O}(\Delta t), \tag{12}$$

where $-1 \le \beta \le 1$ indicates the relative weight of forward versus backward transition probability and $1 < \alpha \le 2$ is the scaling exponent in one-dimensional (1-D) space. The final term $\mathcal{O}(\Delta t)$ indicates higher-order terms that diminish to zero faster than Δt. Since $\exp(-z) = 1 - z + z^2/2 \ldots$, this density contains the expansion for the α stables (including the Gaussian; see section 5) as a subset. A finite variance density requires that $\alpha = 2$, so (12) reduces to the transition density used to derive the classical FPE:

$$\hat{p}(k; \Delta t) = 1 - A(\Delta t)(ik) + B(\Delta t)(ik)^2 + \mathcal{O}(\Delta t), \tag{13}$$

where $2B(\Delta t)$ is equal to the second moment of the particle excursion distances when $\alpha = 2$. This special case instantaneous transition density has an inverse transform that contains derivatives of the Dirac delta function:

$$p(x - \zeta; \Delta t) = \delta(x - \zeta) - A(\Delta t)\delta'(x - \zeta) + B(\Delta t)\delta''(x - \zeta) + \mathcal{O}(\Delta t). \tag{14}$$

This transition density, when substituted into (8), leads to the classical FPE for Brownian motion with advective drift. Power law and α-stable transitions with $\alpha < 2$ have a real-space density for small time (the inverse transform of (12)):

$$p(x - \zeta; \Delta t) = \delta(x - \zeta) - A(\Delta t)\delta'(x - \zeta) + \tfrac{1}{2}(1 + \beta) B(\Delta t) D_+^\alpha \delta(x - \zeta) + \tfrac{1}{2}(1 - \beta) B(\Delta t) D_-^\alpha \delta(x - \zeta) + \mathcal{O}(\Delta t), \tag{15}$$

where $D_\pm^\alpha$ are αth-order fractional derivatives defined in the appendix by equation (A5). The terms involving α-order derivatives can be directly evaluated as proportional to $(|x - \zeta|)^{-1-\alpha}$ (appendix), which shows the power function density of the instantaneous transition approximation. For symmetric jumps, $\beta = 0$. The coefficients $A(\Delta t)$ and $B(\Delta t)$ vanish as Δt goes to zero, as required by (9). We assume that the rate of change of the drift and scale coefficients for small time are constants, so $A(\Delta t)$ and $B(\Delta t)$ are linear with Δt for small transition times, leading to the constants

$$v \equiv \lim_{\Delta t \to 0} \frac{A(\Delta t)}{\Delta t} \tag{16}$$

$$\mathcal{D} \equiv \lim_{\Delta t \to 0} \frac{B(\Delta t)}{\Delta t}. \tag{17}$$

Nonlinear, power function scaling of $A(\Delta t)$ and $B(\Delta t)$ with Δt can be used to model non-Markovian, long-term temporal correlation and leads to a fractional time derivative [*Zaslavsky*, 1994a, b]. For simplicity, we will assume that time correlation is thin-tailed relative to spatial correlation, so that (16) and (17) are good approximations (see also *Benson* [1998] and *Benson et al*. [2000] for evidence of this). Placing the expansion (15) into (8), integrating the delta function term directly, the first-order term by parts, using the integration by parts formula for fractional derivatives (appendix) on the remaining terms, and letting Δt tend toward zero gives a fractional-order FPE:

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x} vP + (\tfrac{1}{2} + \beta/2) \frac{\partial^\alpha}{\partial x^\alpha} \mathcal{D}P + (\tfrac{1}{2} - \beta/2) \frac{\partial^\alpha}{\partial(-x)^\alpha} \mathcal{D}P. \tag{18}$$

The function v is the drift of the process, i.e., the mean advective velocity. If the particle transition is modeled by an infinite variance probability, then the nonlinear growth of the particle propagator is incorporated within the fractional derivative, rather than the leading parameter $\mathcal{D}$. The derivative must be defined so that it correctly captures the scaling of the transition density. The limit in (8) has invoked an ergodic process. The number of individual transitions has become large enough that the (limit) stable distribution results, no matter the specific form of the infinite variance transition density. This constitutes the crux of the applicability of (18): Are a large but finite number of power law transitions (that are bounded by finite velocity) best modeled by a stable law? The limits of this assumption remain an open question, although studies by *Mantegna and Stanley* [1995] and *Makse et al*. [2000] suggest that this is valid over a very large range (number) of transitions.

For a large number of independent solute "particles" the probability propagator is replaced by the expected concentration C [e.g., *Fürth*, 1956; *Bhattacharya and Gupta*, 1990]. Further, since the particle motions are iid, (18) simplifies to

$$\frac{\partial C}{\partial t} = -v \frac{\partial C}{\partial x} + (\tfrac{1}{2} + \beta/2)\mathcal{D} \frac{\partial^\alpha}{\partial x^\alpha} C + (\tfrac{1}{2} - \beta/2)\mathcal{D} \frac{\partial^\alpha}{\partial(-x)^\alpha} C, \tag{19}$$

where the dimensions of $\mathcal{D}$ are $L^\alpha T^{-1}$. For Gaussian or other light-tailed random motions including log-normal, $\alpha = 2$ and the classical ADE is recovered, since $d^2/dx^2 = d^2/d(-x)^2$. The conversion from one to many particles also invokes a slightly different ergodic hypothesis. It assumes that the contaminant is sampling the aquifer as a whole and that the aquifer itself is relatively well mixed. As a result, the quantity C will have dimensional variability in addition to random fluctuations from the mean solution. This has been an area of research in second-order stochastic theory [e.g., *Graham and McLaughlin*, 1989; *Kapoor and Gelhar*, 1994a, b; *Dagan and Fiori*, 1997]. We have not addressed the variability of C around its expected value for the fractional equation.

A special case of the fractional ADE (equation (19)) describes symmetric transitions, where $\beta = 0$. Defining the symmetric operator equivalent to the Riesz potential [*Samko et al*., 1993]:

$$2\nabla^\alpha \equiv D_+^\alpha + D_-^\alpha \tag{20}$$

gives the mass balance equation for advection and symmetric fractional dispersion:

$$\frac{\partial C}{\partial t} = -v \cdot \nabla C + \mathcal{D}\nabla^\alpha C. \tag{21}$$

We use the description "fractional ADE" with the understanding that only the dispersion term is described by a fractional derivative.

4. Solutions of the Fractional Advection-Dispersion Equation

Solutions to common solute transport boundary value problems (BVPs) are gained through Laplace or Fourier transforms in a manner similar to that of *Ogata and Banks* [1961]. Here we solve the BVP for instantaneous injection of a Dirac delta function spike of solute, i.e., the Green function. The fractional-in-space equation (19) is solved via Fourier transform of the fractional derivatives (appendix):

$$\hat{C}(k, t) = \exp\left[\tfrac{1}{2}(1 - \beta)(-ik)^\alpha \mathcal{D}t + \tfrac{1}{2}(1 + \beta)(ik)^\alpha \mathcal{D}t - ikvt\right]. \tag{22}$$

With a notational simplification $\mathcal{B} = |\cos(\pi\alpha/2)|\mathcal{D}$, and the identities $i = e^{i\pi/2}$ and $e^{i\theta} = \cos\theta + i \sin\theta$, we obtain

$$\hat{C}(k, t) = \exp\{-\mathcal{B}t|k|^\alpha[1 + i\beta(\text{sign}(k)] \cdot \tan(\pi\alpha/2)) - ikvt\}. \tag{23}$$

This Fourier transform does not have a closed-form inverse. However, putting it in the form of the characteristic function (substituting $-k$ for k), the density can be manipulated into the canonical form of the characteristic function for α-stable densities (see section 5):

$$\hat{C}(-k, t) = \exp\{-\mathcal{B}t|k|^\alpha[1 - i\beta\ \text{sign}(k) \cdot \tan(\pi\alpha/2)] + ikvt\}, \tag{24}$$

where the positive number $\sigma = (\mathcal{B}t)^{1/\alpha}$ indicates a stable density that is shifted by the mean (vt) and invariant upon scaling by $t^{1/\alpha}$. The entire family of 1-D stable densities is generated from the governing equation, including the Gaussian when $\alpha = 2$. Since different operators describe motions that are faster and slower than the mean, the solutions can include skewness when $\alpha < 2$ (Figure 2). A solution of the simplified, symmetric, fractional advection-dispersion equation (21) results in

$$\hat{C}(k, t) = \exp(-\mathcal{B}t|k|^\alpha - ikvt). \tag{25}$$

It is a simple matter to show that for any $\alpha < 2$, the α-stable variables have infinite variance, since one or both of the tails decay like $f_\alpha(x) \sim c|x|^{-1-\alpha}$ (Figure 3). However, a finite sampling of the density (i.e., a plume) yields a finite sample variance. Since the density is scale invariant with $t^{1/\alpha}$, the sample variance must grow proportional to the square of this. So a plume undergoing Lévy motion would have a sample variance that grows proportional to $t^{2/\alpha}$, or always equal to or faster than Fickian growth.

The solution to the classical ADE with the continuous

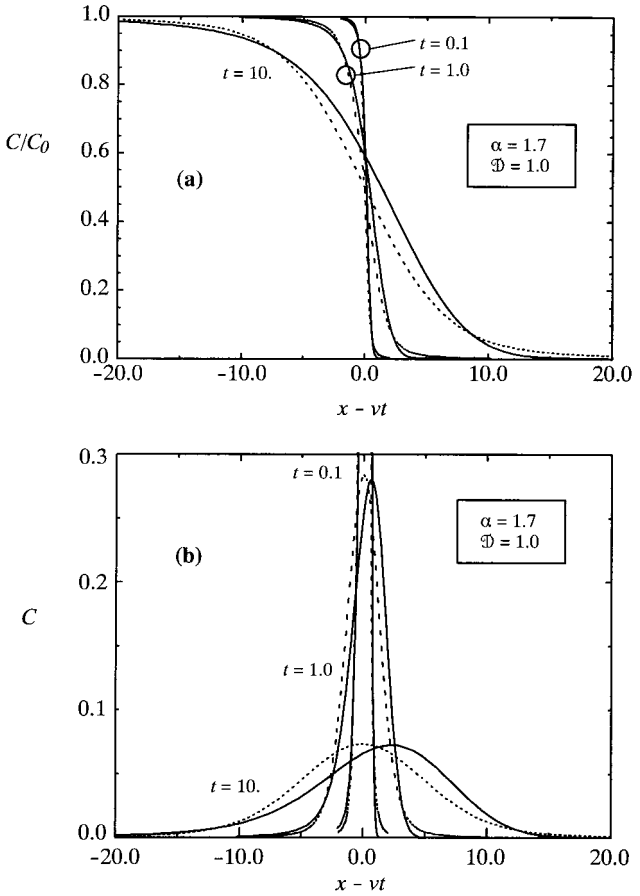

Figure 2. Comparison of the development of spatially symmetric (dashed lines) and positively skewed ($\beta = 1$, solid lines) plumes represented by (a) continuous source and (b) pulse source. Three dimensionless elapsed times (0.1, 1.0, and 10) are shown. As α gets closer to 2, the skewing diminishes. All curves use $\alpha = 1.7$ and $\mathcal{D} = 1$.

source initial condition is generally written in closed form using the error function:

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-x^2}\, dx. \tag{26}$$

This integral has no algebraic formula, so it is numerically estimated and tabulated. The step function BVP using the classical ADE is given by [*Ogata and Banks*, 1961]

$$C = \frac{C_0}{2}\left[1 - \operatorname{erf}\left(\frac{x - vt}{2\sqrt{\mathcal{D}t}}\right)\right]. \tag{27}$$

For continuity with this widely used formula, a similar solution for the fractional advection dispersion equation is given by

$$C = \frac{C_0}{2}\left[1 - \operatorname{serf}_\alpha\left(\frac{x - vt}{(\mathcal{B}t)^{1/\alpha}}\right)\right], \tag{28}$$

where we define the α-stable error function ($\operatorname{serf}_\alpha$) function similarly to the error function, i.e., twice the integral of a symmetric α-stable density from 0 to the argument (z):

$$\operatorname{serf}_\alpha(z) = 2\int_0^z f_\alpha(x)\, dx, \tag{29}$$

where $f_\alpha(x)$ is the standard, symmetric, α-stable density (see section 5). The factor of 2 in the denominator of the $\operatorname{serf}_\alpha$ argument has been dropped from (28) for simplicity. The values of the $\operatorname{serf}_\alpha(z)$ function have been tabulated over a range of arguments from 0 to 10 and for values of α from 1.1 to 2.0 incremented by 0.1 [*Benson*, 1998, Tables 5.1 and 5.2]. Note that the definition of $\operatorname{serf}_\alpha$ (z) uses a standard distribution which, for $\alpha = 2.0$, is a Gaussian with standard deviation of $\sqrt{2}$. Since the error function is a Gaussian with standard deviation of $\sqrt{2}/2$, erf(z) and $\operatorname{serf}_{2.0}(z)$ are related by

$$\operatorname{erf}(z) = \operatorname{serf}_{2.0}(2z). \tag{30}$$

5. Stable Random Variables

DeMoive's CLT for finite variance, iid random variables X_i:

$$\frac{X_1 + X_2 + \cdots + X_n - n\mu}{\sigma n^{1/2}} \Rightarrow Z, \tag{31}$$

where μ and σ are constants, the arrow denotes convergence in probability, and Z is a standard normal random variable, can be generalized by removing the assumption of finite variance [*Lévy*, 1937]:

$$\frac{X_1 + X_2 + \cdots + X_n - n\mu}{\sigma n^{1/\alpha}} \Rightarrow Y, \tag{32}$$

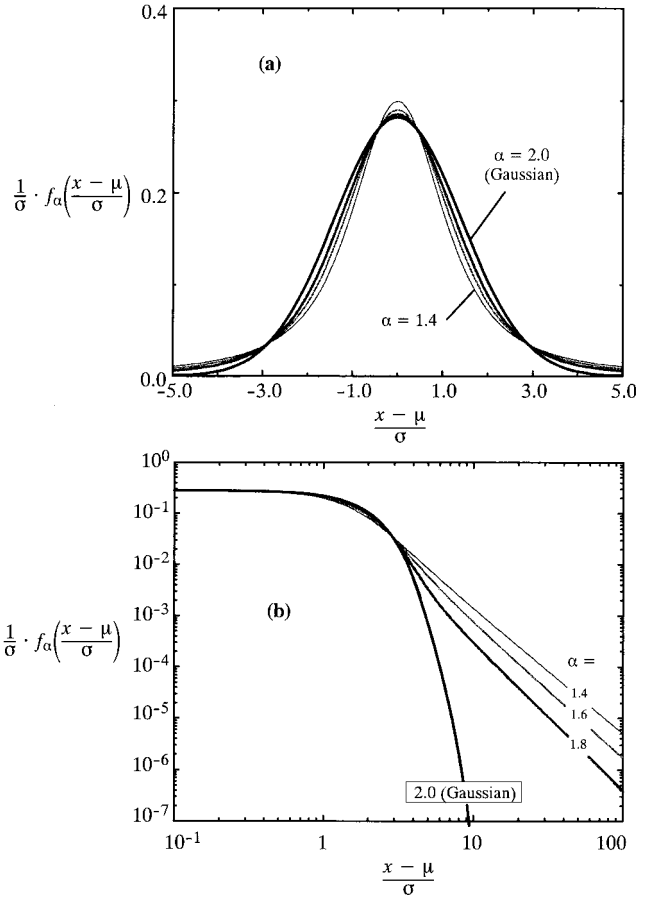

Figure 3. Plots of symmetric α-stable densities showing power law, heavy-tailed character: (a) linear axes and (b) log-log axes.

where Y is a standard α-stable variable that has infinite variance. This is a similar statement to the Fokker-Planck development, with proper rescaling of time via the number of additions of random particle excursions. Densities of α-stable variables are a generalization of the normal probability density function [*Samorodnitsky and Taqqu*, 1994]:

$$\psi(k) = \exp\{-|k|^{\alpha}\sigma^{\alpha}[1 - i\beta \operatorname{sign}(k) \cdot \tan(\pi\alpha/2)] + ik\mu\} \qquad 1 < \alpha \leq 2, \tag{33}$$

where the parameters σ, β, and μ describe the spread, the skewness, and the location of the density, respectively. Equation (33) is the characteristic function (i.e., the Fourier transform with $k \rightarrow -k$ of the probability density function) for stable densities. The sign(k) function is -1 for $k < 0$ and 1 otherwise. The characteristic function for $\alpha = 1$ (the Cauchy distribution) is slightly different from (33) and will not be discussed here for the sake of brevity.

When the density is symmetric, the skewness parameter (β) is zero, and the symmetric characteristic function is

$$\psi(k) = \exp(-\sigma^{\alpha}|k|^{\alpha} + ik\mu). \tag{34}$$

Note the similarity between (34) and (25), the solution to the symmetric fractional advection-dispersion equation. A standard α-stable density function has unit "spread" and is centered on the origin, so $\sigma = 1$ and $\mu = 0$. A nonstandard density $f_{\alpha}(x)$ is related to a standard $s_{\alpha}(x)$ by $f_{\alpha}(x) = \sigma^{-1}s_{\alpha}[(x - \mu)/\sigma]$. A standard, symmetric α-stable distribution is characterized by the compact formula

$$\psi(k) = \exp(-|k|^{\alpha}). \tag{35}$$

In this form, it is easy to see that the Gaussian (normal) density is α-stable with $\alpha = 2$. Note, however, that when the scale factor of the stable law $\sigma = 1$, the standard deviation of the normal ($\alpha = 2$) distribution ($\mathcal{N}$) is $\sqrt{2}$:

$$\mathcal{N}(k) = \exp(-2\sigma^2k^2 + ik\mu). \tag{36}$$

The most important feature of the α-stable distributions (33), (35) is the characteristic exponent (also called the index of stability) α. The value of α determines how "non-Gaussian" a particular density becomes. As the value of α decreases from a maximum of 2, more of the probability density shifts toward the tails. Figure 4 shows the standard α-stable distribution functions for $\alpha = 1.6$, 1.8, 1.9, and 2. Note that the distributions appear very Gaussian in untransformed coordinates and that the difference lies in the relative weight present in the tails. For probabilities between 1 and 99% the different distributions appear near normal; however, the difference between the distributions (the weight in the tails) becomes apparent in probability space (Figure 3b).

Cauchy and Lévy found that direct inversion of the characteristic function $\psi(k)$ to the density function is only possible when $\alpha = 1/2$, 1, or 2. A number of accurate approximations are available for other values. Several series expansions of the standard α-stable densities are listed [*Feller*, 1971; *Nikias and Shao*, 1995; *Janicki and Weron*, 1994]. The density inversion formula also has many real-valued integral representations that yield quick numerical solutions [cf., *Zolotarev*, 1986; *McCulloch and Panton*, 1996; *McCulloch*, 1998; *Nolan*, 1997]. We have used numerical integration (coded in FORTRAN [see *Benson*, 1998, Appendix I]) of McCulloch's integral forms to generate the densities (Figure 3) and distribution functions

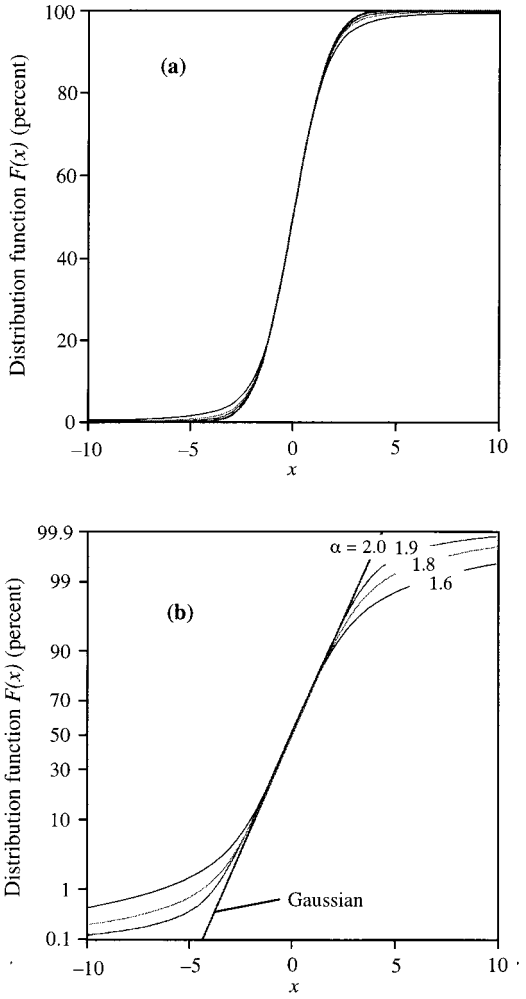

Figure 4. Plots of the distribution function $F(x)$ versus x for several standard symmetric α-stable distributions using (a) linear scaling and (b) probability scaling. The Gaussian normal ($\alpha = 2.0$) plots as a straight line using probability scaling for the vertical axis.

(Figure 4). The constant-source solution of the fractional ADE (Figure 3a) is unity minus the distribution function. The skewness that results from higher probability of particles moving either ahead or behind the mean diminishes as α gets closer to 2.

6. Discussion

The FPE may contain a fractional time derivative [*Giona and Roman*, 1992], which measures the power law random trapping, or "waiting" time that a particle may experience in fractal lattices. *Compte* [1996] showed that power law waiting times and Gaussian trajectories lead to this fractional-in-time diffusion that is typically slower than Fickian. *Zaslavsky* [1994a, b] and *Saichev and Zaslavsky* [1997] suggest that fractional derivatives are allowable in both time and space, resulting in a process similar to fractional Lévy motion [*Saichev and Zaslavsky*, 1997]. *Benson* [1998] showed that a time- and space-fractional equation does not generally follow from coupled power law trajectories and waiting times. He also suggests that such an equation is intractable. *Metzler et al.* [1998] further explore the coupling between fractional time and fractional space processes. *Metzler and Nonnenmacher* [1998] indicate

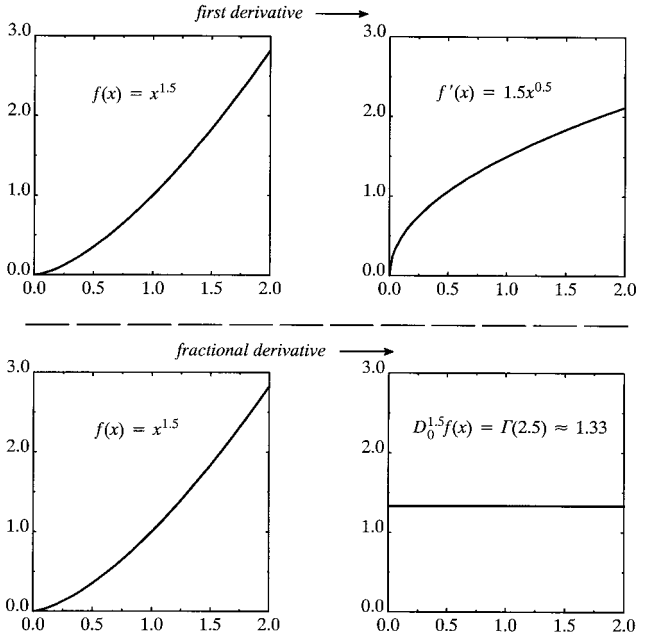

Figure 5. Integer and fractional derivatives of a simple power function. (top) First derivative of $f(x) = x^{1.5}$. (bottom) Fractional derivative around the point $a = 0$ of $f(x) = x^{1.5}$. The first derivative has not reduced the information; that is, the first derivative is still a function of x. The correct fractional derivative reduces the information to a single constant.

that faster-than-Fickian diffusion (or dispersion) is possible with power law waiting times. *Benson* [1998] noted that a fractional time derivative may be useful for the open question of the governing equation for sorbing solutes in heavy-tailed velocity fields.

Several of the derivations that use a fractional space derivative result in special cases. *Zaslavsky* [1994a, b] and *Compte* [1997] use one-sided operators that lead to maximally skewed transitions and limiting stable distributions. *Zaslavsky* [1994a, b] also chose to describe advection with a lower moment ($\alpha/2$) instead of the first. The ($\alpha/2$)-order term leads to a difficult solution that is a convolution of two stable densities. *Compte* [1996] and *Metzler et al*. [1998] use a form that allows only symmetric transitions. *Saichev and Zaslavsky* [1997], *Benson* [1998], *Chaves* [1998], and *Gorenflo and Mainardi* [1998] recognized that two operators are required to generate all possible stable (including symmetric) plumes in 1-D and generate fractional ADEs or diffusion equations similar to (19). *Meerschaert et al*. [1999] generalize spatially fractional dispersion to any number of dimensions after a definition of multidimensional fractional derivatives. They recover all possible stable random vectors. *Gorenflo and Mainardi*'s [1998] intuitive development of a fractional diffusion equation is from an Eulerian, rather than the present LaGrangian, point of view. Finally, *Benson* [1998] shows that the spatial velocity autocorrelation of CTRW that converge to Lévy motion is infinite, but that the same CTRW with upper (largest) cutoff lengths are well approximated by power law autocorrelation.

One way to interpret the simplified form (21) is that a fractional divergence operator is applied to a Fickian dispersion term. For an illustration of how fractional derivatives relate to the definition of divergence in the context of solute transport, consider two simple functions $g(x) = x^2$ and $f(x) = x^{1.5}$. The integer derivatives of $g(x)$ are $g'(x) = 2x$ and $g''(x) = 2$. In the latter case, all of the information about the function is held in a constant. The derivatives deduce how much curvature, or growth, is in a function of another variable by stripping off successive levels of curvature. The integer derivatives describe the curvature of well-behaved (integer-powered) functions but do not fare so well with a rational-powered function. The first or second derivatives of $f(x)$ do not reduced the amount of information needed, since each of these derivatives still depends on (x) (Figure 5). If a fractional differential operator is chosen in which the fractional order of differentiation matches the power law scaling of the function, then the curvature is reduced to a constant, and all of the scaling information is contained in the order of the derivative and that constant. In this case, the 1.5th derivative of $f(x)$ returns a constant (Figure 5). We have used a lower limit of zero in Figure 5 since volume is always nonnegative. If a plume is travelling through material with evolving heterogeneity, then a fractional divergence might account for the increased dispersive flux over a larger range of measurement scale (compare Figures 1 and 5). An open question is whether the fractional operator might incorporate the smallest scale of measurement by using a finite, nonzero lower limit of partial integration (appendix).

7. Conclusions

The fractional advection-dispersion equation is a parsimonious description of particle transport with noninteger space-time scaling. It is based on a Markov process of particle motions that have infinite variance, or heavy-tailed, excursion lengths. The equation is nonlocal in space and describes an ergodic limit process at all times. The Markov process requires that temporal correlation is relatively short-lived, or thin-tailed. Motions that have heavy-tailed temporal correlation may imply a fractional time derivative. Fundamental (Green) function solutions to the fractional ADE developed here are Lévy's α-stable densities. Fickian dispersion is not assumed at any scale. The equation is attractive because, with constant coefficients, it predicts plumes that (1) grow proportional to $t^{1/\alpha}$, (2) have apparent variance that grows proportional to $t^{2/\alpha}$, (3) have heavy leading and/or trailing edges, (4) incorporate any degree of skewness, and (5) are ergodic (limit) processes at all times.

Since the model is based on infinite variance particle excursions, it is perhaps best suited to sites that have heavy-tailed velocity distributions [*Benson et al*., 2000] and very long-range autocorrelation [*Benson*, 1998].

Appendix: Properties of Fractional Derivatives

A number of excellent texts describe the long history and analytical properties of fractional derivatives and fractional differential equations [*Oldham and Spanier*, 1974; *Miller and Ross*, 1993; *Samko et al*., 1993]. Analysis of fractional derivatives is also finding exposure in recent mainstream texts [e.g., *Debnath*, 1995]. Perhaps the most intuitive notion of fractional differentiation is that the Fourier transform of a fractional derivative of order q results in a multiplication in Fourier space by $(ik)^q$. This recovers the integer-order cases when q is any integer. We first list the definitions of fractional derivatives.

The composition rule and the Riemann-Liouville integral give an equivalence between the nearest higher-order integer

and rational order derivatives [*Oldham and Spanier*, 1974; *Miller and Ross*, 1993; *Samko et al*., 1993]. This indicates that fractional derivatives are integer derivatives of "partial integrals." If n is the smallest integer larger than the rational number q, we have

$$D^q_{a+}F(x) = \frac{d^n}{dx^n} I^{n-q}_{a+}F(x)$$

$$= \frac{1}{\Gamma(n-q)} \frac{d^n}{dx^n} \int_a^x (x-\zeta)^{n-q-1} F(\zeta)\, d\zeta, \tag{A1}$$

where $\Gamma(z)$ is the gamma function, which extends the factorial function to real numbers:

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x}\, dx \tag{A2}$$

For values of z between 0 and 1, $1/\Gamma(z)$ is approximately equal to z. The gamma function follows the recursion relationship $\Gamma(z+1) = z\Gamma(z)$. Since $\Gamma(1) = 1$, $\Gamma(n+1) = n!$, where n is an integer.

The lower limit of integration is commonly set to zero or minus infinity. The zero bound is most commonly used for time-dependent functions $u(t)$ that are causal, or nonzero only for $t \geq 0$ [*Giona and Roman*, 1992; *Gorenflo and Mainardi*, 1998]. For spatial functions an infinite bound is typically used, and for notational simplicity the limit is eliminated from the subscript and only the direction of fractional integration (+ or −) is noted.

$$\frac{d^q}{dx^q} f(x) \equiv D^q_+ f(x) = \frac{1}{\Gamma(n-q)} \frac{d^n}{dx^n} \int_{-\infty}^x (x-\zeta)^{n-q-1} f(\zeta)\, d\zeta. \tag{A3}$$

One can integrate from the other side of (x), defining another related type of fractional differentiation [*Samko et al*., 1993] based on integer derivatives of the Weyl partial integral:

$$\frac{d^q}{d(-x)^q} f(x) \equiv D^q_- f(x) = \frac{(-1)^n}{\Gamma(n-q)} \frac{d^n}{dx^n}$$

$$\cdot \int_x^\infty (\zeta - x)^{n-q-1} f(\zeta)\, d\zeta. \tag{A4}$$

Because of their domains of $[-\infty, x]$ and $[x, \infty]$, these are the most useful forms when dealing with functions in physical space. *Samko et al*. [1993] represent both formulas by a single shorthand representation (note the change of (+) to (−) and vice-versa inside the integral):

$$D^q_\pm f(x) = \frac{(\pm 1)^n}{\Gamma(n-q)} \frac{d^n}{dx^n} \int_0^\infty \zeta^{n-q-1} f(x \mp \zeta)\, d\zeta. \tag{A5}$$

Like integer derivatives, a fractional derivative of a power function of x reduces the exponent by the order of the differentiation. With certain restrictions [e.g., *Miller and Ross*, 1993],

$$D^q_{0+} x^u = \frac{\Gamma(u+1)}{\Gamma(u-q+1)} x^{u-q}. \tag{A6}$$

We use the fractional derivative of the Dirac delta function $\delta(x-c)$ with $b \leq c \leq d$, defined by

$$\int_b^d \delta(x-c) f(x)\, dx = f(c). \tag{A7}$$

The fractional derivatives with order $0 < q$ of $\delta(x-c)$ are directly obtained:

$$D^q_+ \delta(x-c) = \frac{1}{\Gamma(n-q)} \frac{d^n}{dx^n} \int_{-\infty}^x \delta(\zeta - c)(x-\zeta)^{n-q-1}\, d\zeta$$

$$= \frac{1}{\Gamma(-q)} \begin{cases} 0 & x < c \\ (x-c)^{-q-1} & x \geq c \end{cases} \tag{A8}$$

and

$$D^q_- \delta(x-c) = \frac{(-1)^n}{\Gamma(n-q)} \frac{d^n}{dx^n} \int_x^\infty \delta(\zeta - c)(\zeta - x)^{n-q-1}\, d\zeta$$

$$= \frac{1}{\Gamma(-q)} \begin{cases} (c-x)^{-q-1} & x \leq c \\ 0 & x > c \end{cases} \tag{A9}$$

By definition, every fractional differential operator is a convolution in either Laplace or Fourier space, depending on the limits of integration. The convolution (asterisk) of functions f and g with respect to Fourier transforms is given by

$$f(x) * g(x) = \int_{-\infty}^\infty g(x-\xi) f(\xi)\, d\xi. \tag{A10}$$

The Fourier transform of a convolution is the product of the transforms of the two functions. We use this property since we require the Fourier transforms of the fractional derivatives. The following result differs slightly from that given by *Debnath* [1995] and used by *Benson* [1998], so we list a brief derivation. The Fourier transform defined by

$$\mathcal{F}[f(x)] \equiv \hat{f}(k) = \int_{-\infty}^\infty e^{-ikx} f(x)\, dx \tag{A11}$$

of integer-order (n) derivatives follows

$$\mathcal{F}[D^n_+ f(x)] = \mathcal{F}\left(\frac{d^n f(x)}{dx^n}\right) = (ik)^n \hat{f}(k) \tag{A12}$$

$$\mathcal{F}[D^n_- f(x)] = \mathcal{F}\left(\frac{d^n f(x)}{d(-x)^n}\right) = (-ik)^n \hat{f}(k). \tag{A13}$$

Starting with the definition of the positive-direction fractional integral (A3) for $n = 0$ and substituting $y = x - \zeta$ gives, for $-1 < p < 0$,

$$D^p_+ f(x) = \frac{1}{\Gamma(-p)} \int_\infty^0 y^{-p-1} f(x-y)(-dy) \tag{A14}$$

$$D^p_+ f(x) = \frac{1}{\Gamma(-p)} \int_{-\infty}^\infty y^{-p-1} H(y) f(x-y)\, dy \tag{A15}$$

where $H(y)$ is the Heaviside function (= 0 for $y < 0$ and 1 for $y > 0$). This is a convolution, which means that the Fourier transform of the left-hand side is equal to the products of the transforms of $x^{-1-p}H(x)/\Gamma(-p)$ and $f(x)$. The former is listed in tables as $|k|^p \exp((i\pi p/2)\ \text{sign}\ (k))$. Since exp

$[(i\pi p/2)\ \mathrm{sign}\ (k)] = i^p$ when $k > 0$ and $(-i)^p$ for $k < 0$, we have

$$\mathcal{F}[D^p_+ f(x)] = (ik)^p \hat{f}(k). \tag{A16}$$

It is a simple matter to show that as the order of the derivative increases (i.e., $n = 1, 2, \ldots$) that the result is general for all orders of fractional derivatives $q = n + p$:

$$\mathcal{F}[D^q_+ f(x)] = \mathcal{F}\{D^n[D^p_+ f(x)]\} = (ik)^n (ik)^p \hat{f}(k)$$
$$= (ik)^{n+p} \hat{f}(k) = (ik)^q \hat{f}(k). \tag{A17}$$

Similar computations for the negative-direction operator give

$$\mathcal{F}[D^q_- f(x)] = (-ik)^q \hat{f}(k). \tag{A18}$$

Finally, the Fourier transforms of the fractional derivatives of a Dirac delta function are

$$\mathcal{F}[D^q_+ \delta(x)] = (ik)^q \qquad \mathcal{F}[D^q_- \delta(x)] = (-ik)^q, \tag{A19}$$

and it follows that a "fractional integration by parts" is similar to the integer-order formula:

$$[D^q_\pm \delta(x)] * f(x) = \delta(x) * [D^q_\pm f(x)] = D^q_\pm f(x). \tag{A20}$$

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