

Operator Lévy motion and multiscaling anomalous diffusion

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The long-term limit motions of individual heavy-tailed (power-law) particle jumps that characterize anomalous diffusion may have different scaling rates in different directions. Operator stable motions $\{Y(t):t \geq 0\}$ are limits of d -dimensional random jumps that are scale-invariant according to $c^H Y(t) = Y(ct)$, where H is a $d \times d$ matrix. The eigenvalues of the matrix have real parts $1/\alpha_j$, with each positive $\alpha_j \leq 2$. In each of the j principle directions, the random motion has a different Fickian or super-Fickian diffusion (dispersion) rate proportional to t^{1/α_j} . These motions have a governing equation with a spatial dispersion operator that is a mixture of fractional derivatives of different order in different directions. Subsets of the generalized fractional operator include (i) a fractional Laplacian with a single order α and a general directional mixing measure $m(\theta)$; and (ii) a fractional Laplacian with uniform mixing measure (the Riesz potential). The motivation for the generalized dispersion is the observation that tracers in natural aquifers scale at different (super-Fickian) rates in the directions parallel and perpendicular to mean flow.

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I. INTRODUCTION

Anomalous diffusion is an important process in hydrogeology because of the way that dissolved and often toxic chemical tracers move through aquifer material. Groundwater velocities span many orders of magnitude and give rise to diffusionlike dispersion (a term that combines molecular diffusion and hydrodynamic dispersion). The measured variance growth in the direction of flow of tracer plumes is typically at a super-Fickian rate, i.e., $\langle (X - \bar{X})^2 \rangle \sim t^{2H}$, where the Hurst index $H > \frac{1}{2}$ [1–7]. A number of theories that are based on the spatial and temporal autocorrelation of the velocity field (or the surrogate hydraulic conductivity K) explain convergence to non-Fickian flux expressions [1–5]. Several of these are based on, or equivalent to, the continuous-time random-walk model [8] and may lead to governing equations with fractional derivatives in time and/or space [2,3,9–11]. These theories are formulated in an isotropic way, so that the scaling behavior and the order of the spatial derivative operator do not vary with direction.

A spatially fractional advection-dispersion equation (ADE) governs an α -stable Lévy motion [12–15], a super-Fickian stochastic process with scaling exponent $H = 1/\alpha$ for some $0 < \alpha < 2$. This equation has been successfully applied to transport in the direction of flow in an aquifer with heavy-tailed K distribution [6]. The order of the space operator and the dispersion (diffusion) coefficient can be discerned from the heavy-tailed K distribution [6] based on an assumption of relatively constant hydraulic gradients and a characteristic correlation time. In many aquifers, the plume also spreads at a super-Fickian rate transverse to the mean flow direction,

indicating a multidimensional anomalous diffusion/dispersion (see Sec. V). The plume is elongated in the direction of flow, indicating anisotropy. Existing models handle anisotropy in the form of a prefactor (usually an effective dispersion tensor) or mixing measure [16–18]. In these models, tracer concentrations may be higher in some directions than others, but the scaling exponent H is the same in every direction. There is no physical reason for this restriction, it is merely a mathematical artifact of the modeling approach. In real aquifer tracer tests, the scaling exponent H usually varies with direction. The rate of spreading is fastest in the direction of flow, and slower (but still possibly super-Fickian) in the horizontal direction transverse to the mean flow. Modeling this behavior requires a new anisotropic model for anomalous diffusion, where the scaling exponent varies with direction. In this study, we extend the spatially fractional ADE to accommodate different scaling exponents in each coordinate. The new governing equation describes an operator Lévy motion, which is a generalization of Lévy motion. This generalized ADE allows a faithful representation of multidimensional tracer plumes, with a faster spreading rate in the direction of the mean flow. Since the physics of diffusion/dispersion is universal, our equation can also be used to model any anomalous diffusion in which the rate of spreading varies with direction.

The term “anomalous diffusion” has been defined in several ways. One standard description requires that a particle in a spreading tracer cloud has a standard deviation that grows like t^H for some $0 < H < 1$, excluding the Fickian case $H = \frac{1}{2}$. This definition is restricted to processes with finite variance, which excludes Lévy motions. Therefore, we choose a definition in terms of $P(x,t)$, the Green function of a diffusive-type equation or the probability density of a particle starting from the origin (the propagator). Super-Fickian

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anomalous diffusion has the space-time scaling property $P(x,t) = t^{-1/\alpha} P(t^{-1/\alpha}x, 1)$ so that the measured standard deviation grows like $t^{1/\alpha}$ for some $0 < \alpha < 2$. Fickian diffusion is the case $\alpha = 2$, where the variance grows linearly with time. Super-Fickian anomalous diffusion is indicated when the classical Fickian diffusion model underestimates the rate of spreading. In this paper, we introduce a generalized diffusion model which includes both super-Fickian and Fickian diffusion as special cases. The novelty of our approach is that we allow the spreading rate to depend on the coordinate. The resulting diffusion can be Fickian in some coordinates and super-Fickian in others, and super-Fickian coordinates can have different scaling. We begin with a review of Brownian motion, Lévy motion, and their governing equations from a statistical mechanical point of view.

II. CLASSICAL ADVECTION AND DIFFUSION

The classical advection-dispersion equation models transport in homogeneous porous media [19]. The same equation, also called the diffusion equation, can be used to describe a wide variety of physical processes [20]. We derive this deterministic governing equation from the scaling limit of a random walk. At a given scale in time and space, we represent the sequence of particle jumps by independent, identically distributed random vectors J_1, J_2, J_3, \dots . The random walk $W(t) = J_1 + \dots + J_{[t]}$ represents the location of a particle at time $t > 0$ at this scale. In a rescaled random walk $c^{-1/2}W(ct)$, a particle takes the random jump $c^{-1/2}J_i$ at time i/c for each integer i . The central limit theorem [21] implies that the probability distributions of this rescaled random walk converge as $c \rightarrow \infty$ to those of a Brownian motion $Y(t)$ with mean zero and covariance matrix tA , assuming that $EJ_i = 0$ and $EJ_i J_i^T = A$. Add a drift with constant mean advective velocity v to obtain $X(t)$ normal with mean tv and covariance matrix tA . If a very large ensemble of independent particles evolves according to this model, the probability density $P(x,t)$ of $X(t)$ represents the relative concentration of particles at location $x \in \mathbb{R}^d$ at time $t > 0$.

According to the random-walk model, after sufficient time has elapsed the relative concentration of diffusing particles will approximate the normal density $P(x,t)$, whose Fourier transform $\hat{P}(k,t) = \exp[-itv \cdot k - (t/2)k \cdot Ak]$. This equation is evidently the solution to an initial value problem

$$\frac{d\hat{P}(k,t)}{dt} = (-v \cdot (ik) + \frac{1}{2}(ik) \cdot A(ik))\hat{P}(k,t)$$

with initial condition $\hat{P}(k,0) \equiv 1$. Invert the Fourier transforms to get the advection-dispersion equation

$$\frac{\partial P(x,t)}{\partial t} = (-v \cdot \nabla + \frac{1}{2}\nabla \cdot A \nabla)P(x,t) \quad (1)$$

whose solution $P(x,t)$ has already been shown to be the family of normal densities with mean vt and covariance matrix tA . The initial condition corresponds to the assumption that $X(0) = 0$.

The advection-dispersion equation (1) describes a tracer cloud whose normalized particle concentration $P(x,t)$ achieves its maximum at the center of mass $x = vt$. For any unit vector θ , the cross section of the plume on a line in this direction through the center of mass follows a normal density with variance $\sigma_\theta^2(\theta) = t\theta \cdot A\theta$. In the isotropic case where $A = aI$, the standard deviation is the same in all directions, so the tracer cloud has rotational symmetry about its mean. For general A , the standard deviation depends on θ , indicating preferential spreading. In any case, $\sigma_\theta^2(\theta) = t\sigma_1^2(\theta)$ for all θ , so that the rate of spreading is at the Fickian rate of $t^{1/2}$ in every radial direction.

III. ANOMALOUS DISPERSION

In real world tracer tests [7,22,23] one typically observes super-Fickian anomalous dispersion, where the plume spreads faster than the classical model predicts. One statistical mechanical derivation of superdiffusion involves a random walk with dependent particle jumps J_i , which can lead to fractional Brownian motion [24]. A mathematically simpler alternative is to retain the assumption of independent jumps, and relax the assumption that the covariance matrix $EJ_i J_i^T = A$ exists. An extended central limit theorem [21,25,26] implies that the probability distributions of a rescaled random walk $c^{-H}W(ct)$ converge as $c \rightarrow \infty$ to those of an α -stable Lévy motion $Y(t)$, where the Hurst index $H = 1/\alpha$ for some $0 < \alpha \leq 2$. The relative concentration of an ensemble of diffusing particles approximates the stable density $P(x,t)$ of the Lévy motion when t is large. Since $P(x,t) = t^{-1/\alpha} P(t^{-1/\alpha}x, 1)$, the tracer cloud spreads out like t^H , faster than the classical model. Sample paths of $Y(t)$ are random fractals [27] of dimension α , so the stable index also has physical meaning, which may relate to the geometric properties of the medium [28]. The particle location $Y(t)$ is a stable random vector [29] with index α . If $\alpha = 2$, we recover the classical Brownian motion model.

The extended central limit theorem applies when the particle jumps J_i have heavy tails. If the random vectors J_i are rotationally symmetric with $P(\|J_i\| > r) \sim Cr^{-\alpha}$, then the limiting process is α -stable with the same kind of symmetry. This leads to the isotropic model of anomalous diffusion, in which a tracer cloud spreads out evenly in all directions from its center of mass at $x = vt$ at the super-Fickian rate $t^{1/\alpha}$. Anisotropic anomalous diffusion results from asymmetric particle jump distributions. Write $J_i = R_i \Theta_i$ and suppose that $P(R_i > r, \Theta_i = d\theta) \sim Cr^{-\alpha} m(\theta) d\theta$ as $r \rightarrow \infty$, where $m(\theta)$ is a probability density on the unit sphere. This means that the probability of a very large jump falls off like $r^{-\alpha}$, and the likelihood of jumping in the direction θ varies proportional to $m(\theta)$. Now the tracer cloud is described by a stable density $P(x,t)$ that is more spread out in some directions than others. This density cannot be expressed in closed form, but when $\alpha \neq 1$ its Fourier transform [18]

$$\hat{P}(k,t) = \exp\left[-ik \cdot vt + ct \int (ik \cdot \theta)^\alpha m(\theta) d\theta\right] \quad (2)$$

solves the initial-value problem

$$\frac{d\hat{P}(k,t)}{dt} = \left[-ik \cdot v + c \int (ik \cdot \theta)^\alpha m(\theta) d\theta \right] \hat{P}(k,t) \quad (3)$$

with $\hat{P}(k,0) \equiv 1$. This inverts to the multivariable fractional advection-dispersion equation

$$\frac{\partial P(x,t)}{\partial t} = (-v \cdot \nabla + c \nabla_m^\alpha) P(x,t), \quad (4)$$

where the operator ∇_m^α is a mixture of fractional directional derivatives [18], so that $\nabla_m^\alpha f(x)$ is the inverse Fourier transform of

$$\left(\int (ik \cdot \theta)^\alpha m(\theta) d\theta \right) \hat{f}(k). \quad (5)$$

When $m(\theta)$ is constant, $\nabla_m^\alpha = \nabla^\alpha$ the Riesz fractional derivative [30], p. 483, recovering isotropic anomalous diffusion. If $\alpha=2$, then $\nabla_m^\alpha = \nabla \cdot A \nabla$, where the matrix $A = (a_{ij})$ with $a_{ij} = \int \theta_i \theta_j m(\theta) d\theta$, recovering classical diffusion/dispersion. The components of $X(t)$ are all scalar Lévy motions with the same index α . If particle jumps are restricted to the coordinate axes, these components are independent, otherwise the dependence is captured by the mixing measure $m(\theta) d\theta$.

IV. GENERALIZED DISPERSION

In both classical and anomalous diffusion/dispersion, normalized particle concentration follows $P(x,t) = t^{-H} P(t^{-H}x, 1)$, where the Hurst index $H=1/\alpha$, so that a cloud of passive tracer particles spreads out from its center of mass like t^H in every radial direction. In real world tracer tests it is commonly observed that the rate of spreading depends on direction [22,23], which requires a generalized model. Since the term t^H scales the vector x , one can also consider matrix scaling. By definition the scalar $t^H = \exp(H \ln t)$. If H is a $d \times d$ matrix, we can also define $t^H = \exp(H \ln t)$, where $\exp(A) = I + A + A^2/2! + A^3/3! + \dots$ is the usual exponential of a matrix. If $H = (1/\alpha)I$, then $t^H = t^{1/\alpha}$ is a scalar multiple as before, but if $H = \text{diag}(h_1, \dots, h_d)$, then $t^H = \text{diag}(t^{h_1}, \dots, t^{h_d})$ so that each coordinate scales at a different rate. The matrix H need not be diagonal. Eigenvalues $a + ib$ induce a rotation at rate $b \ln t$ and degenerate eigenvalues produce terms like $t^a (\ln t)$ in the matrix power t^H .

Generalized diffusion/dispersion is the result of a simple random-walk model with matrix scaling. Since the particle jumps J_i are random vectors, it makes sense to consider the rescaled random walk $c^{-H}W(ct)$, where H is a matrix. Matrix scaling of the random particle jumps $c^{-H}J_i$ accommodates a general pattern of heavy tailed jumps. For example, if the first coordinate of J_i has a finite variance and the second coordinate has a heavy tail which falls off like $r^{-\alpha}$, then we take $H = \text{diag}(1/2, 1/\alpha)$. A generalized central limit theorem [31–33] implies that the probability distributions of the rescaled random walk converge as $c \rightarrow \infty$ to those of an operator Lévy motion $Y(t)$ [34–36]. If $H = \text{diag}(h_1, \dots, h_d)$ with $h_j = 1/\alpha_j$, this requires $0 < \alpha_j \leq 2$. In general, the real parts

of the eigenvalues of H must exceed $\frac{1}{2}$.

Physically, the scaling limit means that an ensemble of diffusing particles will realize the operator stable density $P(x,t)$ when t is large. This density cannot be written in closed form, but when $EX(t) = vt$ its Fourier transform is given by the Lévy representation

$$\hat{P}(k,t) = \exp \left(-itv \cdot k - tk \cdot Ak + t \int (e^{-ik \cdot x} - 1 + ik \cdot x) \phi(dx) \right), \quad (6)$$

where ϕ is the Lévy measure [34,37,38]. The first two terms in Eq. (6) describe a normal distribution, and the last term reduces to the integral in Eq. (2) if $\phi\{\|x\| > r\} = Cr^{-\alpha}$. Because of the sum in the exponential, $\hat{P}(k,t)$ is the product of the normal and heavy-tailed parts, so that these components are independent. For example, if the first coordinate of J_i has a finite variance and the second coordinate has a heavy tail which falls off like $r^{-\alpha}$, the scaling limit has two independent components, one normal and one α -stable. The Lévy measure governs the probability of large jumps, according to $P(J_i = dx) \sim \phi(dx)$ as $\|x\| \rightarrow \infty$ [33]. Since the Lévy measure satisfies $c\phi(dx) = \phi(c^H dx)$ at every scale $c > 0$, the probability of a large jump falls off like a power law depending on direction. If $H = (1/\alpha)I$, then $P(\|J_i\| > r) \sim Cr^{-\alpha}$ and we recover anomalous diffusion. If $H = \text{diag}(1/\alpha_1, \dots, 1/\alpha_d)$, the probability of a large jump in the j th coordinate direction falls off like $r^{-\alpha_j}$, and the j th component of the limit process is an α_j -stable Lévy motion. If particle jumps are restricted to the coordinate axes, these Lévy motions are independent, otherwise the dependence between the coordinate Lévy motions is described by the Lévy measure.

Invert Eq. (6) to see that $P(x,t)$ solves a point source generalized advection-dispersion equation

$$\frac{\partial P(x,t)}{\partial t} = (-v \cdot \nabla + \frac{1}{2} \nabla \cdot A \nabla + \mathcal{F}) P(x,t), \quad (7)$$

where the generalized fractional derivative $\mathcal{F}f(x)$ is the inverse Fourier transform of

$$\widehat{\mathcal{F}f}(k) = \left(\int (e^{-ix \cdot k} - 1 + ik \cdot x) \phi(dx) \right) \hat{f}(k). \quad (8)$$

In real space this means that

$$\mathcal{F}f(x) = \int [f(x-y) - f(x) + y \cdot \nabla f(x)] \phi(dy), \quad (9)$$

which is almost a convolution with the Lévy measure.

The generalized advection-dispersion equation (7) includes both classical and anomalous advection dispersion as special cases. If $1 < \alpha < 2$, the fractional derivative [30]

$$\frac{d^\alpha}{dx^\alpha} f(x) = \frac{1}{\Gamma(2-\alpha)} \int_0^\infty f''(x-y) y^{1-\alpha} dy \quad (10)$$

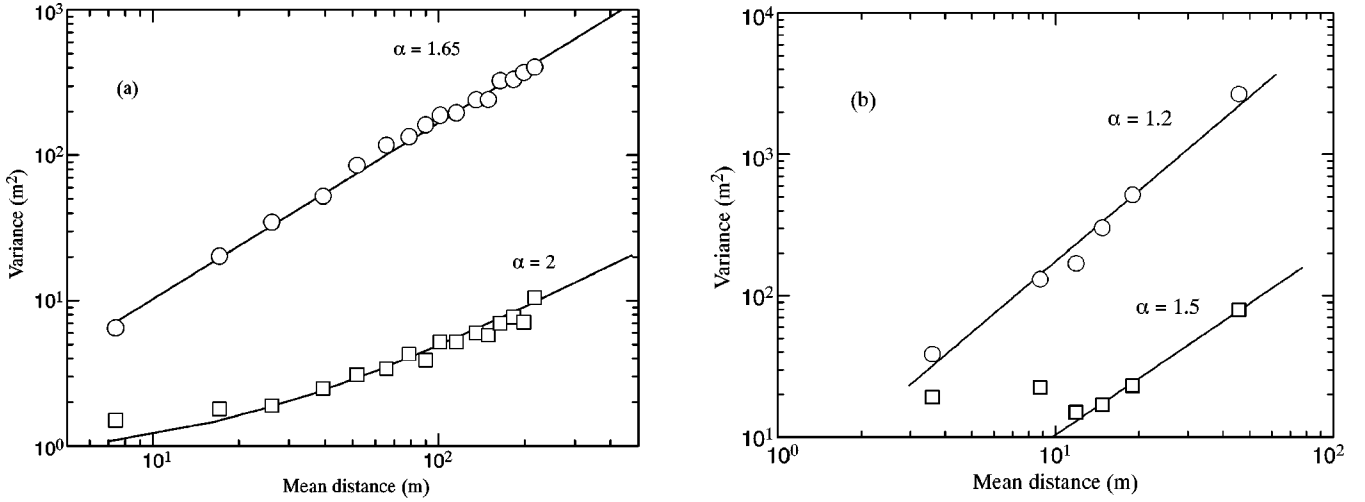


FIG. 1. Measured longitudinal (circles) and lateral (squares) variance of the bromide plumes vs mean travel distance in the (a) Cape Cod [22] and (b) MADE site [23] aquifers. Lines indicate power laws of order $2/\alpha$. Transverse values are artificially high at early time due to the wide (~ 5 m) arrays of injection wells.

and if $\phi(dy) = C\alpha y^{-\alpha-1} dy$ on $y > 0$ integration by parts in Eq. (9) yields

$$\begin{aligned} \mathcal{F}f(x) &= C\alpha \int_0^\infty [f(x-y) - f(x) + yf'(x)]y^{-\alpha-1} dy \\ &= C \int_0^\infty [-f'(x-y) + f'(x)]y^{-\alpha} dy \\ &= \frac{C}{(1-\alpha)} \int_0^\infty f''(x-y)y^{1-\alpha} dy \end{aligned}$$

so that $\mathcal{F} = d^\alpha/dx^\alpha$ if $C = (1-\alpha)/\Gamma(2-\alpha)$. In this case Eq. (7) simplifies to the one-variable fractional diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = -v \frac{\partial P(x,t)}{\partial x} + c \frac{\partial^\alpha P(x,t)}{\partial x^\alpha}$$

which governs a maximally skewed Lévy motion with drift [12,13]. If $\phi(dy) = pC\alpha y^{-\alpha-1} dy$ on $y > 0$ and $\phi(dy) = qC\alpha(-y)^{-\alpha-1} dy$ on $y < 0$, then $\mathcal{F} = pd^\alpha/dx^\alpha + qd^\alpha/d(-x)^\alpha$ and we recover every scalar Lévy motion with drift as the solution to the general one-variable fractional diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = -v \frac{\partial P(x,t)}{\partial x} + cp \frac{\partial^\alpha P(x,t)}{\partial x^\alpha} + cq \frac{\partial^\alpha P(x,t)}{\partial (-x)^\alpha}$$

considered in [14,15]. If $\phi\{\|x\| > r\} = Cr^{-\alpha}$, then $\mathcal{F} = \nabla_m^\alpha$ and Eq. (7) reduces to Eq. (4), which governs multivariable Lévy motion with drift.

The Lévy measure ϕ governs the tails of the particle jumps J_i as well as the fractional derivative operator \mathcal{F} in Eq. (9). Formal integration by parts in Eq. (10) yields

$$\frac{d^\alpha}{dx^\alpha} f(x) = \frac{1}{\Gamma(-\alpha)} \int_0^\infty f(x-y)y^{-\alpha-1} dy, \quad (11)$$

a convolution of generalized functions [39], so that in this case the fractional derivative

$$\mathcal{F}f(x) = \int f(x-y)\phi(dy) \quad (12)$$

is indeed convolution with the Lévy measure $\phi(dy) = y^{-\alpha-1} dy/\Gamma(-\alpha)$ on $y > 0$ in the distributional sense. If $\phi(dy) = p\alpha y^{-\alpha-1} dy/\Gamma(-\alpha)$ on $y > 0$ and $\phi(dy) = q\alpha(-y)^{-\alpha-1} dy/\Gamma(-\alpha)$ on $y < 0$, then Eq. (12) holds with $\mathcal{F} = pd^\alpha/dx^\alpha + qd^\alpha/d(-x)^\alpha$. If $\phi\{\|x\| > r\} = r^{-\alpha}/\Gamma(-\alpha)$, then Eq. (12) holds with $\mathcal{F}f(x) = \nabla_m^\alpha f(x)$. We have not yet been able to compute $\mathcal{F}f(x)$ for matrix scaling, but we conjecture that Eq. (12) still holds in this case.

V. DISCUSSION

Generalized dispersion is an attractive model because it is based on a simple random-walk model. Heavy-tailed (power-law) jumps in d dimensions will converge to the operator stable laws governed by Eq. (6). If independent thin-tailed jumps are mixed with heavy-tailed ones, the index of the heaviest jumps dominates. Granular aquifer material is often deposited in sheetlike to tubelike structures of similar grain size [40]. Fractures in crystalline rock will have preferred directions and lengths [41] according to the external stress field. Many of the transport properties (aperture, displacement, length, connectivity) of natural fractures and faults have power-law distributions and scaling [42–44].

Several tracer tests have been conducted with sufficient sampling detail to resolve anomalous dispersion [22,23]. Two tests show significant differences in the measured variance growth rate in the longitudinal and transverse directions (Fig. 1). In both of the tests, the vertical growth rate was essentially zero, so that the plume growth is two-dimensional. Longitudinal plume dispersion in the relatively homogeneous Cape Cod aquifer is anomalous with $\alpha \approx 1.65$ and Fickian lateral dispersion [Fig. 1(a)]. Here the general-

ized advection-dispersion model resolves into two independent processes, a longitudinal Lévy motion with index α and a lateral Brownian motion. At the highly heterogeneous MADE site, both longitudinal and lateral dispersion are anomalous, but with different scaling [Fig. 1(b)]. The longitudinal $\alpha_1 \approx 1.2$ and the lateral $\alpha_2 \approx 1.5$ so the generalized advection-dispersion model involves a longitudinal Lévy motion with index α_1 and a lateral Lévy motion with index α_2 . The heaviest tail of the MADE plume corresponds to the smallest index α_1 , and this value is consistent with the observed tail index ($\alpha \approx 1.1$) of the hydraulic conductivity (K) random field [6]. An assumption that the hydraulic head gradient was fairly uniform in the longitudinal direction led to a scalar fractional advection-dispersion equation of order 1.1. It may also be possible to obtain *a priori* estimates of the lateral index α_2 based on a model of the K field, which recognizes the possibility of matrix scaling.

VI. CONCLUSIONS

A generalized advection-dispersion equation models transport in porous media, allowing for anomalous diffusion/

dispersion at different rates in each coordinate. This equation governs an operator Lévy motion, the scaling limit of a simple random walk in many dimensions. If the scaling properties are the same in all directions, we obtain the special case of an α -stable Lévy motion, which is governed by a fractional advection-dispersion equation of order α . If the scaling is different in each dimension, we apply a fractional derivative of different order in each coordinate. The resulting operator stable motions may contain independent Brownian motion and Lévy motion components. Detailed plume studies at the Cape Cod and MADE site aquifers show evidence of generalized dispersion, with preferential spreading in the direction of mean flow.

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