Transport and retention in fractured rock: Consequences of a power-law distribution for fracture lengths

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A probabilistic model for the transport of a reacting species in fractured rock is presented. Particles are transported by advection through a series of n rock fractures, and also diffuse and react chemically in the surrounding porous medium. The fracture attributes are unobserved with predefined statistical distribution. The time of arrival t_ϕ of a given fraction ϕ of an initial solute pulse, a key quantity used in a variety of applications, is related to the statistics for fracture apertures and lengths. A classification scheme is developed for the large n asymptotics of t_ϕ. The expected value and variance of t_ϕ are available explicitly if the aperture and length distribution have finite variance. The expected t_ϕ is infinite, and its probability distribution is related to asymmetrical Levy distributions in the case of a power-law distribution for lengths. The most probable time of arrival is proposed as a robust alternative to the expected value. A scaling transition in the most probable t_ϕ versus n is found as the power-law exponent changes. These results suggest that risks associated with migrating contaminants may be misrepresented by conventional stochastic analyses. [S1063-651X(98)10606-2]

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I. INTRODUCTION

Transport through an interconnected network of fractures in an otherwise low-permeability medium is a key issue in subsurface geophysics. Such networks allow contaminants to reach and move through groundwater aquifers, provide transport pathways for radionuclides escaping future deep-rock waste repositories, and affect the recovery of hydrocarbons from fractured reservoirs. Uncertainty about the fracture parameters is an unavoidable issue in these applications, as it is usually not possible to have direct observation of fracture attributes in the subsurface. For this reason, there is great interest in developing probabilistic frameworks for assessing uncertainty and risk [1]. Of particular interest is the time required for solutes to move through a fracture network. Stochastic analysis of this travel time is complicated by microscopic exchange processes which act to retain solutes in the host rock. These include *matrix diffusion*, the process by which particles diffuse into the stagnant water in the pore space of the surrounding rock [2], and physical adsorption and desorption combined with chemical reactions, collectively referred to as *sorption*, which acts to further slow the downstream movement of particles.

Stochastic analysis of transport in fractures is further complicated by the wide distribution of fracture attributes which may be inconsistent with basic assumptions underlying widely used statistical concepts. For example, field studies of fractured rock often support a power-law model for the distribution of fracture lengths l_1 [3], $\Pr\{l_1>s\}\propto s^{-\alpha}$ for large s. In this situation the theoretical moments $\langle l_1^q\rangle$ diverge, and the sample moments are unreliable for $q\geqslant\alpha$. In particular, the length variance is ill defined, and conditions required for the central limit theorem are not met when $\alpha<2$, the situation observed frequently in field studies. Even the mean value is undefined for $\alpha<1$. Although the result of a power-law distribution of lengths is well established empirically, the consequences of this for transport have not been explored.

We propose a stochastic model for transport and retention in fractured rock, and use this model to explore the implications of a power-law fracture length distribution. Most studies of transport in fractured rock rely on continuum-level descriptions for the fracture network and host medium. However, the conditions necessary for employing an effective-medium approximation to the fracture network are often not met in practice. We focus on the opposite limit where the fracture network is barely connected, and transport is confined to highly localized channels or pathways through the network. Transport in this situation is controlled by large-scale fluctuations in advection coupled with the microscopic retention processes, a common situation in environmental systems [4]. Advective transport through the fractures is modeled as a random flight with finite-variance or power-law step distribution. A second random variable correlated with the step size is introduced to control the retention processes.

II. APPROACHES TO MODELING TRANSPORT IN FRACTURED ROCK

Most studies of transport in fractured media rely on continuum-level models derived, for example, via effective-medium theory [5]. This general approach can be extended to include the retention processes of diffusion and sorption by defining two interacting continua, one for the fractures and another for the porous medium. These are referred to as dual-porosity models. More sophisticated versions, the dual-permeability models, allow for flow in both the fractures and the rock matrix. These dual-permeability–dual-porosity models require the fracture density to be large compared to the threshold for percolation. They also require the scale of support for the continuum properties to be large compared to the largest fractures. These situations are often not realized in practice. Moreover, these continuum-level models do not address explicitly the issue of prediction uncertainty, which is of prime interest in contemporary environmental applications.

Hughes and Sahimi [6] described limitations of the dual-continuum models, and developed an alternative lattice model that allows for transport in both pores and fractures and exchanges between the two. They analyzed this model in one spatial dimension and developed an effective-medium approximation. In one spatial dimension, the model in Ref. [6] is unable to describe diffusion controlled exchanges between the fracture and surrounding rock volume. The differential equations describing advection coupled with matrix diffusion can be cast into a lattice form similar to the one in Ref. [6], but two spatial dimensions are required. Moreover, this lattice formulation results in fracture-to-matrix exchange rates that are correlated with the site-to-site transition rates, a situation in conflict with the basic assumptions in Ref. [6]. Finally, the approach does not deal explicitly with prediction uncertainty.

Discrete fracture models constitute another general approach to modeling transport in fractured rock. In this approach, fractures with predefined distributions of aperture, length, and orientation are placed randomly in a simulation domain. Flow and transport can then be calculated for the simulated fracture network. This Monte Carlo approach is useful for site-specific engineering studies.

The approach taken here is similar to the fracture-network simulations in that no attempt is made to define an effective medium. The difference is that we also do not attempt an exact calculation for transport in the multiply connected network. An approximation is considered instead, justified by field results and previous modeling work, that allows for a more generic analysis.

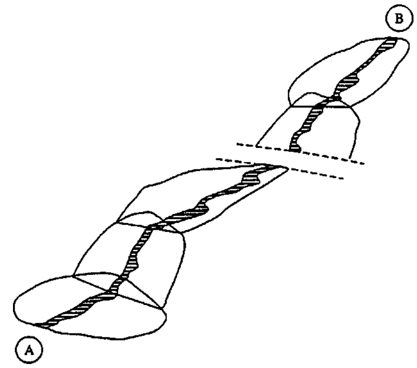

FIG. 1. Conceptual model of a migration pathway for a reacting species in fractured rock. Fluid flowing through a connected series of n rock fractures transports solutes along a streamtube determined by the two streamlines bounding the initial release. Particles diffuse into immobile fluid in the rock surrounding the fractures, where they may also undergo chemical reactions. The streamtube meanders through individual fractures and passes from fracture to fracture as it travels from release point A to outlet B. Branching at fracture intersections is ignored. The streamtube is modeled as a rectangular channel with a piecewise constant aperture and a constant width w_0 set by the size of the initial release. The apertures and lengths for the n fracture segments in the flow path are modeled as independent and identically distributed (IID) random variables.

III. FLOW PATH MODEL

Exact analysis of flow and transport in a fracture networks requires consideration of the multiple routes that particles may take. This complication is why studies using discrete-fracture models rely on Monte Carlo simulation of the fracture networks. Such simulations using field-derived fracture attribute distributions reveal that a small number of transport pathways are often responsible for the majority of the mass flux [7]. Moreover, when the particle source is spatially localized, a single dominant transport pathway is often found. As Sahimi pointed out [5], this is consistent with a barely connected network near the percolation threshold. More important, it is supported by field experiments on tracer transport [8].

Our main simplification is to ignore multiple routes through the fracture network and focus on a single flow path formed by n quasi-two-dimensional fractures connected in series (Fig. 1). This approximation improves as the fracture density approaches the percolation threshold. Other factors improving the quality of this approximation include broad distribution of apertures and lengths, preferred spatial orientation and spatial clustering of fractures, incomplete mixing at fracture intersections, and spatial localization of the particle source.

In most application scenarios, solute particles are released into regions that are small compared to the physical width of a fracture. In the absence of strong dispersion internal to the fracture, particles will not spread out and sample the entire fracture surface, but will be transported along a streamtube determined by the two streamlines bounding the initial release. This is consistent with the flow path model described in [9–11]. Our flow path model, then, consists of a rectangular streamtube with spatially varying aperture $b(x)$ and width $w(x)$, where x is the distance along the streamtube trajectory and $b(x) \ll w(x)$. Water flows through this streamtube at a constant volumetric rate Q. Aperture variability internal to each fracture will cause the width to fluctuate around w_0, the size of the initial release. Fracture-to-fracture variability will also cause the local mean in the aperture to undergo stepwise changes as the streamtube passes from one fracture to the next. For simplicity, we neglect internal variability in fracture apertures relative to fracture-to-fracture variability. The flow path then becomes a sequence of n segments, each with a constant aperture b_i, a random length l_i, and the same width w_0. The goal is to relate the statistics for flux and related quantities at the output of the nth fracture to the probability density function (PDF) for fracture apertures and length.

IV. RETENTION MODEL

Downstream movement of solutes is slowed by diffusion into an essentially immobile fluid in the rock pore space, and by linear equilibrium sorption in the matrix. We neglect, for simplicity, sorption on the fracture surface and concentrate on diffusive effects. If diffusion in the rock matrix is one dimensional without barriers and orthogonal to the fracture plane, the time-dependent flux of solutes at the output of the nth fracture due to a δ function input at the beginning of the first fracture is [10,11]

$$r(t;\tau,\beta)=\frac{H(t-\tau)\kappa\beta}{2\sqrt{\pi}(t-\tau)^{3/2}}\ \exp\left[\frac{-\kappa^2\beta^2}{4(t-\tau)}\right]. \tag{1}$$

Here $H(\ )$ is the unit step function, $\kappa=\theta\sqrt{DR_m}$, θ is the matrix porosity, $R_m=1+K_d^m$, K_d^m is the distribution coefficient for sorption in the matrix, and D is the coefficient of diffusion into the rock matrix.

The random variable τ is the residence or transit time for advection, and the new random variable β controls the rate of diffusion and surface sorption. The macroscopic random variables τ and β in Eq. (1) are

$$\tau=\frac{1}{Q}\int_0^l w(x)b(x)dx=\sum_1^n \tau_i\simeq\frac{1}{q}\sum_1^n l_ib_i,$$
$$\beta=\frac{1}{Q}\int_0^l w(x)dx=\sum_i^n \beta_i\simeq\frac{1}{q}\sum_1^n l_i, \tag{2}$$

where $q=w_0/Q$, and $l=\Sigma_i^n l_i$ is the total length along the trajectory. The approximations in Eq. (2) apply within the context of our piecewise constant approximation to the flow path.

The time of arrival of a cumulative mass fraction ϕ is an important quantity in environmental applications. Its value relative to the half-life for radionuclide decay or chemical degradation is particularly important when considering migrating contaminants. It is calculated from Eq. (1) as

$$t_\phi=\tau+\eta\beta^2. \tag{3}$$

If t_ϕ and τ are actual times, then $\eta=\kappa^2/4F^2$, where $F(\phi)$ is the inverse complementary error function. If t_ϕ and τ are normalized by τ_0, the characteristic time for nonreactive transport in a single fraction, and β by $\beta_0=l_0/q$, then $\eta=\kappa^2\beta_0^2/4F^2\tau_0$ is dimensionless and contains all the deterministic model parameters. This result is useful in its own right as it provides a simple method for quick evaluation of the importance of retention processes relative to advection. This could be used, for example, in comparing the suitability of various candidate sites for nuclear waste repositories. We consider this normalized form and retain the same symbols. How the characteristic time is defined depends on the single-fracture distributions. If the expected values exist, this would be a good choice.

V. STOCHASTIC ANALYSIS

The cumulative arrival time t_ϕ is a random quantity due to its dependence on the random quantities τ and β, which in turn depend on the random apertures and lengths. If the length or aperture moments exist, they can be related to the moments t_ϕ, thus providing a simple method for calculating the quantities required in applications based on quantities estimated in field studies. Specific results and examples can be found in [12].

In the situation of a power-law distribution for lengths, $\langle\beta^2\rangle$, and thus the expected value for the arrival time $\langle t_\phi\rangle$, becomes infinite if matrix diffusion is present ($\kappa\neq 0$). This is caused by long tails in the length distribution, and should not be confused with spatial localization. Physically, particles have a small but significant probability of encountering fractures with long residence times and large β. These rare fractures dominate the ensemble averages and render sample statistics unreliable. The implications are fundamental: if fracture lengths have a power-law distribution, then the common practice of calculating expected values and variances in the predicted arrival times of contaminants may be unreliable, and should be replaced with more robust measures that are less sensitive to tails of the distribution.

One alternative to moment analysis is to calculate the full probability density function (PDF) for t_ϕ

$$f_{t_\phi}(t_\phi)=\int_0^\infty f_{\beta,t_\phi}(\beta,t_\phi)\ d\beta=\int_0^\infty f_{\beta,\tau}(\beta,t_\phi-\eta\beta^2)d\beta. \tag{4}$$

For independent and identically distributed (IID) fractures, the density $f_{\beta,\tau}$ is related to that of the individual fractures f_{β_1,τ_1} by an n-fold convolution

$$\tilde{f}_{\beta,\tau}(\nu,\omega)=[\tilde{f}_{\beta_1,\tau_1}(\nu,\omega)]^n, \tag{5}$$

where $\tilde{f}_{\beta,\tau}$ is the fourier transform of $f_{\beta,\tau}$. Using our piecewise constant approximation to the flow path, $\beta_i=l_i/q$, $\tau_i=b_il_i/q$, and

$$f_{\beta_1,\tau_1}(\beta_i,\tau_i)=\frac{q}{\beta_i}f_{l_1,b_1}\left(\beta_iq,\frac{\tau_i}{\beta_i}\right). \tag{6}$$

Equations (4)–(6) do not depend on specific assumptions about the τ_1,β_1 distribution or even the existence of moments of the distribution. These can be used to compute the PDF of arrival times based on the joint PDF of fracture length and aperture. Examples will be explored in a future publication [12]. Here we concentrate on generic results such as the large n asymptotics.

VI. ASYMPTOTIC SCALING

In the absence of mass transfer, $\kappa=0$, and Eq. (1) is a δ function, i.e., a particle injected at the first fracture will arrive at the output of the nth fracture after time τ. This situation corresponds to a random walk of n steps, with duration for the steps governed by $f_{\tau_i}(\tau_i)$. Here τ_i is the advective residence time for a single fracture. Basic results on random walks can be used to deduce the probability density for t_ϕ at large n in this situation. Specifically, $f_{t_\phi}(t_\phi)$ will tend to a Gaussian if the individual steps are IID with finite second moment, and to an asymmetrical Levy-stable distribution if the IID steps have an infinite-variance power-law distribution (see, e.g., Ref. [13]). When retention processes are included, similar results are obtained for the large n distribution of β and τ for use in Eq. (4).

In order to explore the consequences of a power-law distribution more clearly, we neglect the variability in the fracture aperture and fix the aperture at a value b_0 for all fractures in the pathway. Although the transmissivity of fractures is known to be sensitive to the size of the fracture aperture, this is not an issue in the present situation because the volumetric flow rate Q is held constant instead of the applied pressure gradient. With aperture fixed, a power-law distribution for length implies the same for τ_1, $f_{\tau_1}(\tau_1) \simeq A_0 \alpha \tau_1^{-\alpha-1}$ for large τ_1. Using our normalization, $b_0=1$, $f_{\tau,\beta}(\tau,\beta)=f_\tau(\tau)\delta(\tau-\beta)$, and

$$f_{t_\phi}(t_\phi)=\zeta^{-1} f_\tau\left(\frac{\zeta-1}{2\eta}\right), \tag{7}$$

where $\zeta=\sqrt{1+4\eta t_\phi}$.

Although sums of IID power-law variables are not covered by the central limit theorem, they do have a corresponding limit theorem. Specifically, sums of IID power-law variables tend to the Levy-stable distributions [14,15] as n becomes large. Using Eq. (7) and the generalized central limit theorem [15] for one-sided power-law variables, we have the following approximation for large n:

$$f_{t_\phi}(t_\phi) \simeq \zeta^{-1} C_n^{-1} \psi\left(C_n^{-1}\left[\frac{\zeta-1}{2\eta}-d_n\right];\alpha,1,0,1\right), \tag{8}$$

where $\psi(\cdot;\alpha,C,d,a)$ is the density for a Levy-stable distribution with levy index α, width C, location parameter d, and asymmetry parameter a. Here the width parameter is given by

$$\frac{nA_0}{C_n^\alpha}=\begin{cases}\Gamma(1-\alpha)\cos(\pi\alpha/2), & 0<\alpha<1\\ 2/\pi, & \alpha=1\\ \dfrac{\Gamma(2-\alpha)}{\alpha-1}|\cos(\pi\alpha/2)|, & 1<\alpha<2.\end{cases} \tag{9}$$

where $\Gamma(\ )$ is the gamma function. The location parameter in Eq. (8) is

$$d_n=\begin{cases} nd_1, & 0<\alpha<1\\ nC_n\langle \sin(\tau_1/a_n)\rangle, & \alpha=1\\ n\langle\tau_1\rangle, & 1<\alpha<2,\end{cases} \tag{10}$$

where the probability density for τ_1 is confined to the half-line $\tau_1>d_1$ when $0<\alpha<1$. Equation (8) holds in the limit $n\to\infty$. The quality of the approximation at finite n depends on the initial distribution of single-fracture residence times. If, for example, $f_{\tau_1}(\tau_1)=\psi(\tau_1;\alpha,C_1,d_1,1)$ then Eq. (8) is exact for all n.

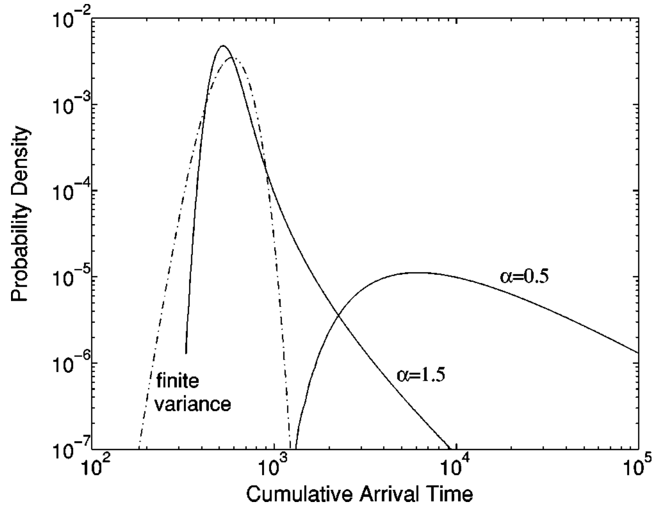

FIG. 2. Probability density for normalized time of arrival t_ϕ of the cumulative mass fraction ϕ at the output of the 50th fracture. The results shown are for $\eta=0.22$ and three different fracture length distributions: a finite-variance distribution and power-law distributions with exponents $\alpha=0.5$ and 1.5. The large n PDF for t_ϕ is very different for the different length distributions.

Shown in Fig. 2 is $f_{t_\phi}(t_\phi)$ for different length (or τ_1) distributions. The solid curves were obtained from Eq. (8) using $\alpha=1.5$ and 0.5. The dashed curve was obtained by assuming a finite-variance distribution. These results are for $n=50$, and the limit distributions are assumed to be adequate approximations. The mean residence time is $\langle\tau_1\rangle=1$ for the $\alpha=1.5$ and the finite-variance cases. In the absence of diffusion, t_ϕ would peak near $n\langle\tau_1\rangle=50$. The shift to longer times is caused by the retention processes. The mean residence time is not defined for $\alpha=0.5$. In this case we used $d_1=1$. There are significant differences in $f_{t_\phi}(t_\phi)$ for the three cases. Density for the $\alpha=0.5$ case peaks at much later times, and the distribution is much broader. The differences between the finite-variance case and the $\alpha=1.5$ case are also significant, especially for early and late arrivals. In particular, the finite-variance distribution predicts higher probability for early arrival of the contaminant mass. Applications involving migrating contaminants are particularly sensitive to early arrivals as this determines the probability of arriving before significant decay has occurred. These results suggest that finite-variance models may be overestimating risk in some situations.

The main feature of Fig. 2 is that the probability density for t_ϕ peaks near the same value for the finite-variance and $\alpha=1.5$ cases, but at much later times for the $\alpha=0.5$ case. The location of this peak, $\tau_\phi^\star$, which is the most probable value of the arrival time, scales differently with n depending on the sign of $\alpha-1$. To see this note that the prefactor ζ^{-1} in Eq. (8) is a relatively slowly varying function of t_ϕ, compared to the Levy-stable density which is strongly peaked. Thus the location of the maximum in the Levy-stable density determines $t_\phi^\star$ approximately,

$$t_\phi^\star=\frac{[(C_n x_\star+d_n)2\eta+1]^2}{4\eta}-1, \tag{11}$$

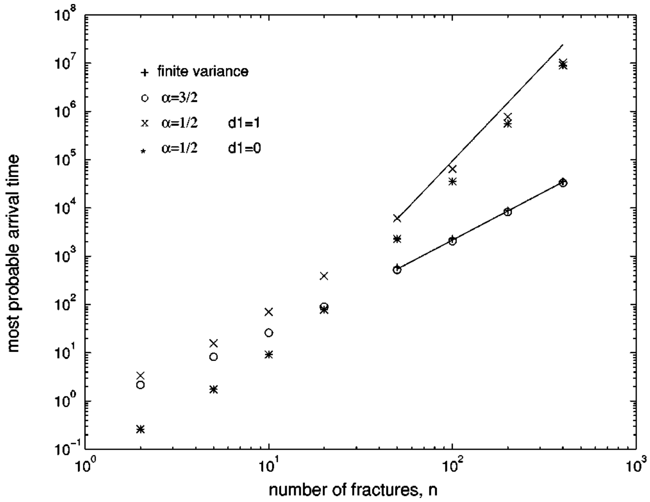

FIG. 3. Most probable time of arrival $t^\star_\phi$ for cumulative mass fraction ϕ vs number of fractures n for power-law and finite-variance distributions for fracture length. The solid lines are the approximate relations in Eq. (12). The same asymptotic scaling is obtained for $t^\star_\phi$ vs n in the finite-variance case and $\alpha=1.5$ power-law case, but a very different scaling is obtained when $\alpha=0.5$. Here α is the power-law exponent (Levy index), and d_1 is the minimum allowed value for fracture length, which is used in place of the expectation value for length when $\alpha\leqslant 1$.

where $x_\star$ is defined implicitly through $\psi'(x_\star;\alpha,1,0,1)=0$. C_n and d_n scale differently with n depending on α. For large n the C_n term will dominate over the d_n term if $\alpha<1$. The converse is true for $\alpha>1$. This leads to the following approximations for large n,

$$t^\star_\phi \simeq \begin{array}{ll} \eta\langle\tau_1\rangle^2 n^2, & \alpha>1 \\ C_1^2\eta x_\star^2 n^{2/\alpha}, & \alpha<1. \end{array} \qquad (12)$$

Similar arguments for the finite-variance situation produce the same scaling as in the power-law $\alpha>1$ situation.

In Fig. 3 we show $t^\star_\phi$ versus n using four different assumptions on the τ_1 distribution. The solid lines are Eq. (12) for $\alpha=1.5$ (lower line) and 0.5 and the individual data points were obtained by numerically locating the maximum in f_{t_ϕ} [16]. The different scaling with n for the different α predicted by Eq. (12) is clear. Equation (12) overestimates $t^\star_\phi$ by about a factor of 2 for $\alpha=0.5$, but gives a good approximation to the asymptotic scaling. The $\alpha=1.5$ and finite-variance examples closely approximate each other as predicted. These results show that, as far as $t^\star_\phi$ is concerned, the important distinction to make when analyzing field data is between the $\alpha<1$ and $\alpha>1$ situations. Misinterpreting a power-law distribution with $\alpha>1$ as a finite-variance distribution with a long tail will not result in serious error in the predicted $t^\star_\phi$. Such a misinterpretation will, however, misrepresent the prediction uncertainty.

VII. CONCLUSIONS

In summary, we developed a stochastic model for transport in fractured rock. This model treats advection as a random flight through fracture segments. Retention in the surrounding rock is also modeled stochastically using a second macroscopic random variable representing the area available for diffusion from the fracture to the host rock. Statistics for the arrival time of a given mass fraction are developed in terms of the statistics for length and aperture, thus providing simple alternatives to complex numerical simulations used in applications. Fundamentally different behaviors are found depending on whether the fracture lengths have finite-variance or power-law distributions.

The proposed classification scheme for the asymptotics of $t^\star_\phi$ versus n has important implications in probabilistic assessment of risk associated with contaminant migration in fractured rock. Applying probabilisitic methods appropriate for finite-variance distributions may result in a serious misrepresentation of the underlying risk. It is thus important to make the distinction between a distribution with long tail and finite-variance distribution as opposed to a power-law distribution when analyzing subsurface data. Using $t^\star_\phi$ as the characteristic value for the arrival time instead of $\langle t_\phi\rangle$ is more robust, but it is still important to distinguish between the $\alpha>1$ and $\alpha<1$ situations. These results clearly demonstrate the importance of exploring alternatives to classical statistical models for natural systems.

Finally, we point out that there is no general solution to the problem of reactive transport in fractured media, as the results depend on the type of mass transfer and chemical processes occurring within the host medium. Our results apply to the situation of unlimited diffusion and equilibrium sorption in the host matrix. However, the approach used, a bivariate random walk with one variable controlling advection in fractures and the other controlling the microscopic retention processes, may be of more general methodological interest for similar problems with more complex chemical reactions in the host rock.

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