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Fickian dispersion is anomalous

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SUMMARY

The thesis put forward here is that the occurrence of Fickian dispersion in geophysical settings is a rare event and consequently should be labeled as anomalous. What people classically call anomalous is really the norm. In a Lagrangian setting, a process with mean square displacement which is proportional to time is generally labeled as Fickian dispersion. With a number of counter examples we show why this definition is fraught with difficulty. In a related discussion, we show an infinite second moment does not necessarily imply the process is super dispersive. By employing a rigorous mathematical definition of Fickian dispersion we illustrate why it is so hard to find a Fickian process. We go on to employ a number of renormalization group approaches to classify non-Fickian dispersive behavior. Scaling laws for the probability density function for a dispersive process, the distribution for the first passage times, the mean first passage time, and the finite-size Lyapunov exponent are presented for fixed points of both deterministic and stochastic renormalization group operators. The fixed points of the renormalization group operators are p-self-similar processes. A generalized renormalization group operator is introduced whose fixed points form a set of generalized self-similar processes. Power-law clocks are introduced to examine multi-scaling behavior. Several examples of these ideas are presented and discussed.

1. Introduction

Starting about 55 years ago (Zwanzig, 1960), people in the physics community began to recognize that diffusive processes are often non-Fickian, i.e., what people now label as anomalous. Back in the day, in an Eulerian frame and in Fourier–Laplace space, non-Fickian was synonymous with a wave vector and/or a frequency dependent diffusion tensor. Since the wave vector is dual to space and frequency is dual to time, this is equivalent in real space to a space and/or time dependent diffusion tensor which is all too often imbedded as a kernel in an integro-partial differential equation (Cushman and Ginn, 1993; Cushman et al., 1994; Neuman, 1993; Neuman and Tartakovsky, 2009; Berkowitz et al., 2002). It is well known and almost a classical result, that mathematically this "non-locality" is a manifestation of upscaling in a heterogeneous environment. See Koch and Brady (1987) or Gelhar and Axness (1983) for early observations of this phenomenon in porous media. Interest in non-Fickian dispersion in hydrogeology was spurred by the MADE tracer tests (Boggs et al., 1992), which concerned field-scale transport. More recently, numerical simulations of flow and transport in detailed pore-spaces imaged from geologic media have continued to generate interest in anomalous transport, but at a much smaller scale (e.g., Blunt et al., 2013; Kang et al., 2014). It is indeed odd that in view of how long people have recognized that dispersion/diffusion may be anomalous (Gelhar et al., 1992) that most introductory texts on hydrogeology and even many more advanced texts on ground water contamination, do not even consider that dispersion might not be Fickian—it is dogma.

In a Lagrangian frame, a process is considered Fickian provided the mean square displacement is linear in time, otherwise the process is considered anomalous or non-Fickian. Often researchers delineate dispersive regimes by a power law mean square displacement classification scheme: $\langle (X(t)-X(t))^2\rangle \sim t^{\alpha}$, if $\alpha > 1$ then the process is called super dispersive, if $\alpha < 1$ then the process is called sub dispersive, otherwise it is called Fickian, Brownian or classical.

The main goal of this short communication is to argue that Fickian dispersion is an anomaly, and that what people label as anomalous dispersion is in reality the norm. In so doing we will also illustrate some major problems with the power law classification mentioned above. We will also review an alternative

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classification scheme based on a renormalization group analysis and related scaling laws for self-similar mixing processes.

2. Fickian/Brownian dispersion/diffusion

In an Eulerian frame, to say a process is Fickian means the dispersion tensor is constant in time, i.e. does not depend on how long you watch the mixing process. For simplicity in our discussion, and to illustrate our most important points, we will also assume it does not depend on space. Further, we assume a conservative tracer is being observed. The Fokker–Planck equation for such a process takes the form

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

where C is the normalized concentration or transition density and D is the constant dispersion tensor. Without loss of generality we assume the medium is isotropic so that the dispersion tensor is diagonal and further we align the x-direction along the direction of mean flow. Thus there are two distinct components of D, longitudinal and transverse, D_L and D_T respectively.

Corresponding to the Eulerian Eq. (1), in two dimensions with the velocity constant and aligned in the x-direction, there are two Lagrangian stochastic ode's

$$\begin{aligned} &dX(t) = V_x dt + \sqrt{D_L} dB_x(t) \\ &\text{and} \\ &dY(t) = \sqrt{D_T} dB_y(t) \end{aligned} \tag{2}$$

where dB_x and dB_y are independent Brownian motions for the trajectory of a particle $(X(t), Y(t))$. Mathematically, a Brownian motion is defined by three points:

(1) The process is continuous and at the origin initially.
(2) The process has independent and weakly stationary increments.
(3) The increments, $X(t) - X(s)$, are Gaussian, $N(0, t-s)$, $t > s$.

Violation of any of these points gives rise to a non-Fickian process, i.e., a process that will not satisfy Eqs. (1) or (2).

3. Types of Non-Fickian dispersion

Historically, non-Fickian (anomalous) dispersion has been categorized in a Lagrangian framework as super-, sub-, or classical (Fickian) by employing a power-law, mean-square displacement (MSD) analogy: Let the MSD be a power law of the form $\langle (X(t) - X(0))^2 \rangle \sim t^\alpha$. If $\alpha > 1$ the process is said to super-dispersive, if $\alpha < 1$ the process is sub-dispersive and it is Fickian if $\alpha = 1$. The case of infinite second moment is also considered super dispersive in this scheme. As will be illustrated shortly, though not widely understood, this classification is fraught with difficulty. But before we illustrate why it is a poor classification scheme, we wish to dispel some widely held beliefs about the causes of anomalous dispersion.

The following quote is in a very popular paper (Metzler and Klafter, 2000): A power law MSD "is intimately connected with a breakdown of the central limit theorem, caused by either broad distributions or long range correlations". The fact that this is not the case is demonstrated by the following simple counter example (Cushman et al., 2009). Consider a Brownian motion $X(t) = B(H(t))$ that is run with a deterministic, but non-linear and absolutely continuous clock, $H(t)$, that is non-negative with derivative $h(t)$. It is not hard to see that the increments, $X(t) - X(s)$ are $N(0, H(t) - H(s))$. A discrete random walk that represents this process is given by $X(tn/M) - X(t(n-1)/M) \sim N(0, h(tn/M)t/M)$. The classical central limit theorem applies to this walk and shows its convergence to $X(t)$, yet if one sets $H(t) = t^\alpha$, $\alpha \neq 1$, then one has $\langle X^2(t) \rangle = t^\alpha$ which is non-Fickian dispersion. There are no broad distributions (the increments are Gaussian) and no long range correlations (the increments are independent) in this example. What makes this counter example work is the non-stationary increments.

This last example begs the question: Mathematically what are the origins of non-Fickian dispersion? The answer is provided in the following (O'Malley and Cushman, 2012a): Let $X(t)$ have zero mean with independent wide-sense stationary increments such that $\langle [X(t) - X(0)]^2 \rangle = f(t) < \infty$, then one can show that $f(t) = ct$ for some constant c. Thus for a power-law mean square displacement to occur, the process must have either increments that are not independent or increments that are not wide-sense stationary. Keep in mind that a process with stationary and independent increments can still be non-Fickian if the increments are non-Gaussian. The essential problem with classifying diffusive processes based on their MSD alone is that this statistic does not provide enough information to distinguish between dispersive processes that are fundamentally different.

Two simple examples (O'Malley and Cushman, 2012a) will illustrate the problems with the MSD classification scheme. The first is a process that has infinite MSD, but by any reasonable measure, is sub-dispersive. The second is an uncountable number of processes that have linear MSD, but that are anything but Fickian. These counter examples rely on the non-linear clock introduced earlier.

Let $X(t) = L_\alpha(1/[1 + \exp(-t)] - 1/2)$ where $L_\alpha(t)$ is an α-stable Levy motion. An α-stable Levy motion is like a Brownian motion except the Gaussian distribution for increments is replaced with a heavy tailed α-stable distribution. The non-linear clock in this example is $G(t) = 1/[1 + exp(-t)] - 1/2$. The process can be simulated by setting $X(0) = 0$, and accumulating increments using the rule that $X(t) - X(s) \sim S_\alpha([G(t) - G(s)]^{1/\alpha}, \beta, 0)$ where $S_\alpha(\sigma, \beta, \mu)$ is an α-stable random variable with spread parameter σ, skewness parameter β, and shift parameter μ. Because $L_\alpha(t)$ has infinite second moment, so does $X(t)$, yet as illustrated in Fig. 1 this process comes to a screeching halt and hence should be considered sub-dispersive. This occurs because the limit of $X(t)$ as t goes to infinity is the limit of $L_\alpha(t)$ as t approaches 1/2 from the left. Since α-stable Levy motion has limits on the left, the limit exists and the trajectory eventually becomes mired in a small neighborhood of the limit.

Next let $X(t) = B_H(t^{1/2H})$ where $B_H(t)$ is a fractional Brownian motion with Hurst exponent H and non-linear clock $G(t) = t^{1/2H}$. A fractional Brownian motion is like a Brownian motion except the increments are $N(0, (t-s)^{2H})$ where $0 < H < 1$ is known as the Hurst exponent. When run with this non-linear clock the MSD takes the form $\langle X(t)^2 \rangle = t$. Realizations of this process appear in Fig. 2. Thus the MSD power law classification would suggest this is Fickian process; yet it is anything but Fickian. Except when H is 1/2 this process is non-Markovian with fractal dimension 2-H (the fractal dimension is a measure for the space-filling ability of the trajectory). Brownian motion has fractal dimension 3/2. Fractional Brownian motion has been used extensively in geohydrology to model non-Fickian transport and distributions of hydraulic conductivity (e.g., Molz et al., 1997; Benson et al., 2013; Dempsey et al., 2015).

4. The scarcity of Fickian processes

By its' very construction, the Lagrangian trajectory that gives rise to Fickian dispersion has weakly stationary increments. Yet it has recently been shown that stationary increment processes are mathematically extremely rare, and many researchers have experimental evidence to suggest that weakly stationary processes