Application Of Stochastic Methods To Creating Models Of Contaminant Transport And Dispersion In Rivers And Groundwater

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Abstract: Purely stochastic methods can yield useful prediction models of contaminant arrival-time distributions derived from advective-dispersive transport in a variety of one-dimensional environments. Two different models are considered, both relating to dispersion of a brief pulse of conservative contaminant in a steady flow system. The first model considers the arrival-time of a contaminant pulse in a river channel with hydraulic interaction with an adjacent unconfined aquifer (hyporheic zone). The contaminant particles experience chance delays in the hyporheic zone where all particle movement is deemed to be at right angles to the channel. This model is mathematically equivalent to a one-dimensional random walk with positive, zero, or negative drift. Zero drift yields scale-invariant arrival-time distributions, with all other drift values giving inverse Gaussian arrival times. Negative drift implies some contaminant particles never escape the hyporheic zone. The case of zero or near-zero drift is of particular interest because the arrival-time distribution is then characterized by long $t^{-3/2}$ tailing over considerable time ranges. This gives a possible explanation of a recent river tracer experiment which recorded power-law tailing over a long period. The second dispersion model considers the case of temporal moments of contaminant arrival-time distributions when flow is partitioned into parallel stream tubes with independent advection-dispersion within each stream tube. This includes, for example, perfectly stratified aquifer systems or river systems where some flow moves along old linear channel deposits. This model yields the general result that the *r*th temporal central moment is an *r*th order polynomial function of contaminant travel distance. For example, the arrival time variance is a quadratic function of contaminant travel distance. This relation holds independently of arrival-time distributions and variations of hydraulic conductivity across the stream tubes.

Keywords: *Modeling; Inverse Gaussian, Hyporheic zone; Stratified aquifer; Temporal moments*

1. INTRODUCTION

Simple stochastic techniques can be useful tools for approximating the behaviour of contaminant transport in natural hydrological environments. This paper considers two variations on a theme of modeling a contaminant arrival-time distribution given one-dimensional transport and dispersion of a brief pulse of conservative contaminant under conditions of steady flow and spatial homogeneity in the transport direction.

2. RIVER DISPERSION WITH SUB-CHANNEL WATER EXCHANGE

2.1. Introduction

The first model presented here is motivated by a recently-reported investigation where a mountain stream tracer experiment exhibited long t^{-k} power-law tailing of tracer arrival time at an observation site downstream from the tracer input point (Haggery et al. 2002). The tailing effect was attributed to variable tracer delay in the stream hyporheic zone where stream water penetrates the unconfined aquifer beneath and lateral to the channel bed.

Haggerty et al. (2002) utilised a weighted mixture distribution which gives rise to t^{-k} tailing over a certain range of t. This model is somewhat empirical, however, in that k is an unknown parameter which must be estimated from data. That is, their model does not anticipate any specific small value of k which would give rise to long-tailing tracer behavior like that observed in their experiment. Motivated by the need for a more specific predictive model, the section below describes a stochastic transport model which has the prediction advantage of including $t^{-3/2}$ power-law tailing over varying time durations which may extend to infinity as a special case.

2.2. Model description

The basic geometric structure of the model is similar to that of Cvetkovic and Haggerty (2002), with particle transport between a tracer release point and a downstream observation point being modeled as a random walk on a one-dimensional lattice with equidistant nodes. The step length between adjacent nodes along the river channel is defined in the present model to be the distance Δx, where Δx is assumed to be small relative to the distance between the tracer release and observation points.

The model has a second spatial dimension in that there is a possibility that any one channel node can divert a particle into an alternative one-dimensional random walk at right angles to the channel transport direction (Figure 1). This represents the model of a particle visitation to the hyporheic zone where, for this model, the particle can only move perpendicular to the original transport direction. As with the channel nodes, the nodes on hyporheic zone random walks are spaced equally and are separated by the small distance increment Δy, which may be small relative to Δx.

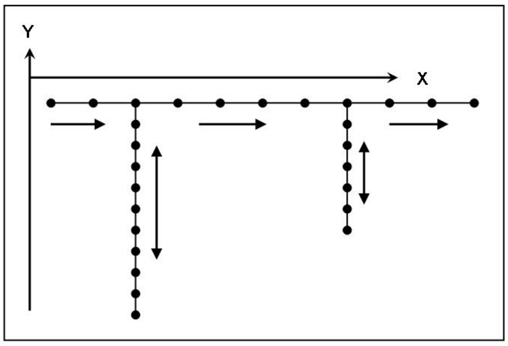

Figure 1. Schematic of the channel random walk model with possible diversion to the sub-channel hyporheic zone. Channel particles step from left to right in the x direction, with chance diversion at right angles from the channel nodes. Two possible diversions of a single random walk are shown.

A contaminant particle starts at the x-origin at time zero. From a given channel node, the particle either steps to the next channel node to the right (with probability p) or is diverted with probability q to the next node in the negative y direction and enters the hyporheic zone A particle in the hyporheic zone can only move either to the next node in the positive y direction (with probability p) or to the next node in the negative y direction (with probability q). The time taken for a particle to step between adjacent nodes is taken to be constant, regardless of whether the step distance is Δx or Δy. If $p \geq 0.5$ then the walk will eventually terminate at the downstream observation point. For $p < 0.5$ there is a finite probability that the particle will never return to the original channel departure site and will thus remain permanently in the hyporheic zone.

As far as arrival times at the observation point are concerned, the above description is mathematically equivalent to a simple random walk on a line from a particle release point to an absorbing barrier at the observation point In this case p and q respectively indicate probabilities of a step to the left or right.

2.3. Model arrival-time distributions

Because Δx is small the equivalence of the diversion process to a simple one-dimensional random walk allows arrival-time limit results to apply, as given by Folks and Chhikara (1978) and associated discussion of that paper. Specifically, for $p \neq 0.5$ the arrival-time distribution follows approximately an inverse Gaussian distribution which can be parameterised:

$$f(t) = \left(\frac{\mu\delta}{2\pi t^3}\right)^{1/2} e^{\delta} \exp\left[-\tfrac{1}{2}\delta\left(\tfrac{t}{\mu}+\tfrac{\mu}{t}\right)\right] \quad (1)$$

$$t, \mu, \delta > 0$$

where μ is the distribution mean and δ is a shape parameter.

For $p < 0.5$ the inverse Gaussian distribution applies to particles which reach the observation point in finite time (Whitmore, 1978). For $p = 0.5$ the arrival-time distribution corresponds to the first passage time of drift-free Brownian motion (Kingman, 1978). Rather than using Kingman's parameterisation, this distribution is parameterised here by its modal value as:

$$f(t) = \left(\frac{3\xi}{2\pi t^3}\right)^{1/2} \exp\left(-\frac{3\xi}{2t}\right) \quad \xi,\, t > 0 \quad (2)$$

$$F(t) = 2\Phi\left[-\left(3\xi/t\right)^{1/2}\right] \quad (3)$$

where $f(t)$ and $F(t)$ are respectively the density functions and distribution functions, ξ is the density function modal value, and Φ is the standard normal integral.

The zero-drift distribution (2) is characterized by a long right tail (Figure 2), has infinite mean and variance, and a finite median of 6.58ξ. The distribution is scale-invariant in that the shape of the distribution remains unchanged as the distance between the origin and the absorbing barrier increases. Scale-invariant properties have implications for environmental analysis and impose some restrictions on environmental information, as noted by Haggerty et al. (2002).

It is evident from inspection of (1) that for δ sufficiently small there will be a tail region of the inverse Gaussian distribution where the probability density will decline as $t^{-3/2}$. That is, the log of $f(t)$ will plot linearly against log(t) with gradient -3/2. This gradient extends to infinity for the special limit case of the zero-drift distribution. The extending linear gradient segment with decreasing inverse Gaussian shape parameter δ is illustrated in Figure 3, with the zero-drift distribution having the limit linear form.

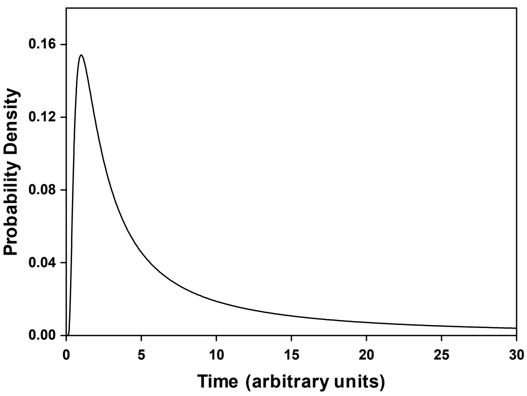

Figure 2. Plot of the zero-drift arrival-time distribution (2) for ξ =1.

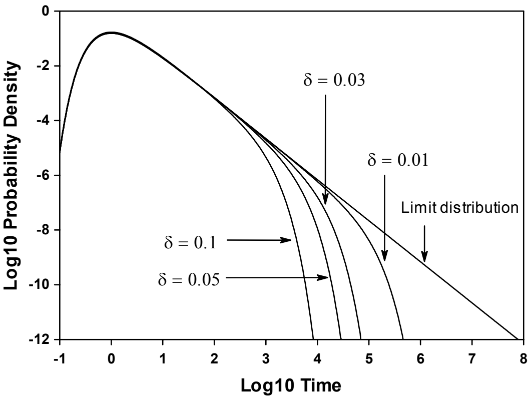

Figure 3. Double-log plot of the inverse Gaussian distribution (1) for a mode of 1.0, showing linear -3/2 tailing increasing as the shape parameter δ decreases. The limit distribution refers to (2) with a mode of ξ = 1.0.

2.4. Discussion and application

The model described above gives an explanation for contaminant arrival-time power law tailing as $t^{-3/2}$. This represents a special case of the arrival-time model and there is no particular physical reason to anticipate the drift parameter will in general be near zero to produce $t^{-3/2}$ tailing. Rather, the model suggests that if long tailing is present then a -3/2 gradient is to be anticipated. Arrival-time tailing as $t^{-3/2}$ is also predicted for the special physical situation of single-rate matrix diffusion – see, for example, (Hadermann and Heer, 1996). The present model is rather more general, however, in that no detailed geometric constraints such as spherical matrix material is required. Observed $t^{-3/2}$ tailing therefore cannot in itself be taken as evidence of a single-rate matrix diffusion process.

Haggerty et al. (2002) recorded tracer data over 3.5 days and estimated a k value of 1.28 from data subsequent to 1.5 hr, which was defined as the initiation of approximate log-linearity. However, there is some scope for variation in the k estimate which changes a little with the choice of time of onset of log-linearity. For example, subsequent to 8 hr the k estimate increases to 1.48 (Figure 4). It is difficult to say whether this estimate is more accurate, but there is scope for a reasonable match of most of the data set to the theoretical k value of 3/2.

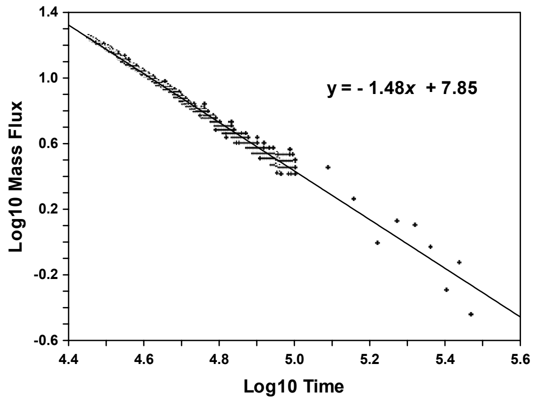

Figure 4. Least-squares regression line fitted to the data of Haggerty et al. (2002), subsequent to 8 hr from the initiation of recording, showing the linear gradient estimate of -1.48.

A feature of the model discussed here is that particles exit from the hyporheic zone at the same point at which they entered. The present model is not therefore a general model of hyporheic zone transport because such zones may in fact be quite mobile in the sense of having flow paths in the direction of river flow over a considerable range of distance scales (Kasahara and Wondzell, 2003). However, the long-tailing ability of the present model does indicate that multi-scale hyporheic flow is not a prerequisite for generating long arrival-time tails from tracer experiments in river systems with groundwater interaction.

3. TEMPORAL MOMENTS FOR PARALLEL FLOW SYSTEMS

3.1. Introduction

Parallel flow models provide a convenient representation of one-dimensional contaminant dispersion by groundwater movement in aquifers with significant stratification, or in sub-river systems where there may be preferential flow paths along old channels. The concept is that water flow moves independently in some arbitrary number of independent stream tubes. The basic model of a parallel flow system for contaminant transport analysis is shown in Figure 5. There is a conceptual input plane which introduces a contaminant pulse into all the stream tubes simultaneously. These individual pulses then move in isolation until some discharge plane is reached after travel distance *x* where the contaminant contributions are mixed and the mixed concentration is monitored over time as an arrival-time distribution.

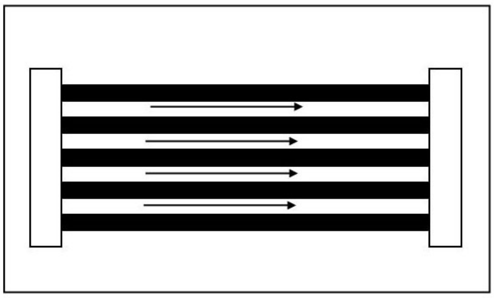

Figure 5. Schematic of isolated parallel stream tubes where contaminants are introduced at a vertical input surface on the left and emerge at a vertical mixing surface on the right (after Rasmuson, 1985).

The concept of parallel groundwater flow systems dates at least to the work of Mercado (1967) who used a perfectly stratified aquifer model of purely advective tracer dispersion. There have been a large number of recent publications dealing with aspects of the contaminant arrival time distribution for the parallel model under various specific conditions. Part of these investigations have been directed toward the moments of the arrival-time distribution, or “temporal moments”.

To date, however, there have been no results presented of a simple temporal moment relation as a function of the parallel flow travel distance *x*, given arbitrary advective-dispersive transport in each stream tube. This section is concerned with the derivation of such a relation by way of using the standard moment relations of a finite mixture distribution model.

3.2. Derivations

It is evident that a system of stream tubes will generate a flux-weighted arrival-time distribution consisting of a finite mixture of the component arrival time distributions generated by the individual stream tubes. Without loss of generality, an equivalent model can be formulated in terms of a system of *N* stream tubes with equal contaminant fluxes. The mixture arrival-time distribution can then be written as the unweighted finite mixture distribution:

$$g(t,x) = N^{-1}\sum_{i=1}^{N} f_i(t,x) \tag{4}$$

where $g(t,x)$ is the arrival-time distribution and the component $f_i(t,x)$ distributions are the arrival-time distributions specific to the respective stream tubes. The required temporal moment distance expressions can therefore be obtained from the moments of the finite mixture distribution (4).

Under advective-dispersive contaminant transport, the cumulant ratios of the component $f_i(t,x)$ distributions will remain constant and independent of *x*. Omitting the *i* subscript for now, define the set of cumulant ratios Z_r of a single $f(t,x)$ distribution as:

$$Z_r = \kappa_r / \kappa_1 = \kappa_r / \mu_1' \quad r \geq 2 \tag{5}$$

where μ_1' is the first moment about zero (distribution mean), and κ_r is the *r*th cumulant of the component distribution concerned. Because the Z_r values are constant cumulant ratios, they are independent of μ_1' and hence are independent of tracer travel distance x.

In general, any distribution’s *r*th moment about zero (μ_r') can be written as a function of the distribution cumulants. For the second, third, and fourth moments about zero, these expressions are, respectively:

$$\mu_2' = \kappa_2 + \kappa_1^2 \tag{6}$$

$$\mu_3' = \kappa_3 + 3\kappa_2\kappa_1 + \kappa_1^3 \tag{7}$$

$$\mu_4' = \kappa_4 + 4\kappa_3\kappa_1 + 3\kappa_2^2 + 6\kappa_2\kappa_1^2 + \kappa_1^4 \tag{8}$$

The corresponding expressions in terms of Z_r and μ'_1 are obtained from (6), (7), and (8) by substituting κ_r with $Z_r \mu'_1$ (for $r \geq 2$), and substituting κ_1 with μ'_1, giving:

$$\mu'_2 = Z_2 \mu'_1 + \mu'^2_1 \tag{9}$$

$$\mu'_3 = Z_3 \mu'_1 + 3 Z_2 \mu'^2_1 + \mu'^3_1 \tag{10}$$

$$\begin{aligned} \mu'_4 &= Z_4 \mu'_1 + (4 Z_3 + 3 Z_2^2) \mu'^2_1 \\ &+ 6 Z_2 \mu'^3_1 + \mu'^4_1 \end{aligned} \tag{11}$$

In the context of a given $f(t,x)$ distribution, it is evident from (9), (10), and (11) that the distribution moments about zero are evidently polynomial functions of μ'_1, and therefore of *x*.

Turning now to the parallel flow system as a whole and reintroducing the *i* subscript, define t and t_i respectively as random variables generated from $g(t,x)$ and $f_i(t,x)$, and define:

$$\phi = E(\mathrm{t}) \tag{12}$$

$$\phi \alpha_i = \mu'_{1\,i} = E(\mathrm{t}_i) \tag{13}$$

where the α_i values in (13) are constants independent of x. This constancy of the α_i values arises because each stream tube has its own constant flow speed, causing each $E(\mathrm{t}_i)$ to remain in constant ratio with $E(\mathrm{t})$.

Define $\mu'_{r\,i}, \mu_{r\,i}$, and $\kappa_{r\,i}$, respectively, as the *r*th moment about zero, *r*th central moment, and *r*th cumulant, of $f_i(t,x)$. Similarly, μ'_r and μ_r are the *r*th moment about zero and *r*th central moment of $g(t,x)$.

As noted in (5), the cumulant ratios specific to each $f_i(t,x)$ are defined:

$$Z_{r\,i} = \kappa_{r\,i} / \mu'_{1\,i} \qquad r \geq 2 \tag{14}$$

and the *r*th moment about zero of $g(t,x)$ is the mean of the component distribution moments about zero:

$$\mu'_r = N^{-1} \sum_{i=1}^{N} \mu'_{r\,i} \tag{15}$$

It follows from (9)-(11) that the corresponding moments of $g(t,x)$ about zero can be expressed (omitting the summation range for brevity):

$$\mu'_2 = N^{-1} \left(\phi \sum Z_{2\,i} \alpha_i + \phi^2 \sum \alpha_i^2 \right) \tag{16}$$

$$\mu'_3 = N^{-1} \left(\begin{aligned} &\phi \sum Z_{3\,i} \alpha_i + 3\phi^2 \sum Z_{2\,i} \alpha_i^2 \\ &+ \phi^3 \sum \alpha_i^3 \end{aligned} \right) \tag{17}$$

$$\mu'_4 = N^{-1} \left(\begin{aligned} &\phi \sum Z_{4\,i} \alpha_i \\ &+ \phi^2 \sum (4 Z_{3\,i} + 3 Z_{2\,i}^2) \alpha_i^2 \\ &+ 6\phi^3 \sum Z_{2\,i} \alpha_i^3 + \phi^4 \sum \alpha_i^4 \end{aligned} \right) \tag{18}$$

The corresponding central moments of $g(t,x)$ can now be obtained by substituting the $g(t,x)$ moments (16)-(18) into the standard statistical expressions giving distribution central moments as functions of moments about zero. This yields the first four central moments of $g(t,x)$ as simple polynomial functions of mean travel time ϕ. These expressions are lengthy and are not reproduced here. However, after gathering constants the arrival-time central moment expressions, to *r* = 4, can be compactly represented as the polynomial in ϕ:

$$\mu_r = \sum_{n=1}^{r} \beta_n \phi^n \tag{19}$$

where μ_r is the *r*th central moment of the arrival-time distribution and the β_n terms are constants independent of ϕ. This polynomial relation presumably holds for all positive integer *r*, subject to the existence of the *Z* ratios.

Because ϕ is proportional to tracer travel distance x, it is evident from (19) that the *r*th central moment of $g(t,x)$ varies as an *r*th order polynomial function of both x and ϕ. This result is general for parallel flow systems in that it holds for any $N \geq 2$, for any arbitrary set of $f_i(t,x)$ distributions which possess finite moments, and for arbitrary independent advective-dispersive transport in the respective stream tubes.

3.3. Discussion

It can be shown that the polynomial coefficients in (19) are all positive for the special case of μ_2, which is the arrival-time variance. That is, the arrival-time variance increases as a quadratic function of contaminant travel distance. It is well known that such a quadratic relation holds for purely advective transport in the stream tubes, so (19) generalises this result to arbitrary advective-dispersive transport in the stream tubes as well.

The higher-order arrival-time moments may be associated with both positive and negative coefficients in their respective polynomial functions. This raises the possibility of higher-order polynomials with a number of turning points with the implication of considerable changes in arrival-time distribution form as travel distance increases. For example, there may be changes in the sign of skewness of arrival-time distributions with increasing *x*.

4. CONCLUSIONS

Basic stochastic models and statistical methods can yield useful insights into the contaminant transport process in natural hydrological environments. Such approaches should be fully investigated prior to the application of complex models of spatial heterogeneity.

With respect to the two models considered here, the simple random-walk model gives a useful specific prediction of $t^{-3/2}$ power law tailing of long-tailed contaminant arrival-time distributions. This provides a logical first check in the analysis of such data. The finite-mixture model also makes a useful contribution in providing a compact representation of the distance evolution of arrival-time central moments in that the *r*th central moments is an *r*th order polynomial function of travel distance, as given by (19). To the author's knowledge, (19) has not been presented previously in the literature of contaminant dispersion in parallel flow systems.

5. ACKNOWLEDGEMENT

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