The tempered one-sided stable density: a universal model for hydrological transport?

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Abstract
A generalized distribution for the water residence time in hydrological transport is proposed in the form of the tempered one-sided stable (TOSS) density. It is shown that limiting cases of the TOSS distribution recover virtually all distributions that have been considered in the literature for hydrological transport, from plug flow to flow reactor, the advection–dispersion model, and the gamma and Levy densities. The stable property of TOSS is particularly important, enabling a seamless transition between a time-domain random walk, and the Lagrangian (trajectory) approach along hydrological transport pathways.

Keywords: hydrological transport, water residence time, statistical distribution

1. Introduction
Quantifying water residence time (WRT) $\tau$ distributions in hydrological transport is important in a wide range of environmental applications, from pollution risk assessment [11], to a basic understanding of biogeochemical processes on the catchment scale [9]. WRT distributions and fluxes provide an important basis for contaminant transport in groundwater [41, 5, 6, 14] as well as in surface water networks [35, 36, 17, 18], however, quantifying WRT distributions for the coupled surface–subsurface flow system still poses a significant challenge [10, 25].

Hydrological transport is difficult to quantify due to a wide variety of structures and dynamic flow conditions that are encountered in the hydrosphere, from complicated drainage networks and macro-porous soil, to heterogeneous aquifers and random discrete structures in fractured rock. As a consequence of this complexity, a relatively wide range of transport models in the form of WRT distributions have been used for interpreting tracer data. A comprehensive study of a series of neighboring catchments in Wisconsin (USA), for instance, explores WRT distributions such as the exponential distribution, the gamma distribution and plug-flow model and their combinations [26]. Other studies emphasize the applicability of the gamma distribution for WRT in catchments [27, 15, 12, 20], use the exponential distribution [19, 37, 17, 26], explore the advection–dispersion model as a way of interpreting WRT observations [22], or advocate anomalous transport models [39].

Given the complexity of the problem and the variety of distributions used for modeling WRT in hydrological systems, the question is whether one can identify a general statistical model of WRT such that in the limit the variety of models from the literature can be recovered as special cases. It is the aim of this paper to propose a generalized statistical distribution of WRT for hydrological transport and demonstrate its relation to a variety of existing models.

2. The tempered one-sided stable density
Water transport takes place along flow paths or trajectories for which the spatial scale can be defined. Whereas the flow velocity may change in time, the flow pattern is assumed to be steady state.

Let $\tau [T]$ denote the WRT along a flow path (trajectory) between two given locations, for a given starting time. If the flow path is appropriately segmented with specified segment
lengths $\Delta x_i$, the key issue is to quantify the statistically independent transition times $\Delta \tau_i$. Let the density for $\Delta \tau$ be stationary and defined in the Laplace transformation (LT) domain as

$$\hat{\psi}(s) = \exp[c_i(a_i^\alpha - c_i(a_i + s)^\alpha)]$$

(1)

where $s$ is the LT variable, and the parameters $a_i$ and $c_i$ are defined as

$$a_i = \frac{1 - \alpha}{\Delta \tau_i \zeta_i^2}, \quad c_i = \frac{\Delta \tau}{\alpha a_i^{\alpha - 1}}$$

(2)

$a_i$ is the cut-off rate, $\Delta \tau$ is the mean and $\zeta_i$ is the coefficient of variation of $\Delta \tau$, and $0 < \alpha < 1$ is an exponent.

Computation of WRT along a trajectory composed of $N$ segments is obtained by convolution:

$$\hat{f}(s) = \prod_{i=1}^N \hat{\psi} = \exp[ca^\alpha - c(a + s)^\alpha]$$

(3)

where $c = \sum c_i$ and $a = a_i$ are conditions of stability; in other words, the cut-off rate $a$ is the same for segment and trajectory WRT, whereas $c$ scales as a sum over all segments. The conditions of stability also imply that the mean and variance for segments and for the entire trajectory, scale in the same manner, i.e. $\text{Var}[\Delta \tau_i]/\text{Var}[\tau] = \Delta \tau/\bar{\tau}$, where $\text{Var}[\Delta \tau]$ is the segment variance, and $\text{Var}[\tau]$ the trajectory variance with $\tau = \sum \Delta \tau$.

3. Limiting cases

Virtually all densities used for travel (residence) times in hydrological transport, from plug flow to a flow reactor, are obtained as limiting (special) cases of the TOSS density. In table A.1 we show the correspondence and limiting TOSS parameters, which yield the various distributions. The proof for the gamma distribution is provided using moments (see the appendix); the exponential distribution is a special case of the gamma distribution.

4. Properties

We shall illustrate the TOSS properties in relation to various WRT densities common for hydrological transport. A convenient parametrization of the densities is based on the mean and coefficient of variation of WRT $\tau$, i.e. $\bar{\tau}$ and $\zeta = \sqrt{\text{Var}[\tau]/\bar{\tau}}$ (table A.1).

The two parameters $a$ and $c$ are illustrated as functions of $\zeta$ and $\alpha$ in figure 1, for a wide range of dispersion, from $\zeta = 1$ to 100, with the exponent $\alpha$ spanning $0 \leq \alpha \leq 1$ in intervals of 0.1. Increasing $\zeta$ (dispersion) decreases the cut-off rate significantly following a simple linear pattern on a log–log plot (figure 1(a)). The parameter $c$ also decreases with increasing $\zeta$, however the pattern is more complex depending on $\alpha$. For $\alpha = 1$ (plug flow, thick blue line in figure 1(b)), $c$ is independent of $\zeta$ (since dispersion is zero) and $c = \bar{\tau}$. With increasing $\alpha$ up to 0.5 (advection–dispersion model, red line), $c$ decreases with $\zeta$ at an increasingly larger rate (figure 1(b)). For the limit $\alpha \rightarrow 0$ (gamma distribution, green line in figure 1(b)), $c$ decreases most rapidly with $\zeta$. Clearly, with increasing $\zeta$ and $\alpha \rightarrow 0$, convergence to anomalous transport is observed.

In figure 2, the cumulative distribution function (CDF) (figure 2(a)) and complementary cumulative distribution function (CCDF) (figure 2(b)) of the TOSS distribution are illustrated for $\zeta = 1.2$, including the limiting cases. The most dramatic differences are in the early arrival (figure 2(a)), where the 0.1% fractional arrival times for the gamma distribution ($\alpha \rightarrow 0$, cyan line) and the plug-flow limit ($\alpha \rightarrow 1$, black dotted line) differ by four orders of magnitude. The interval $0 < \alpha < 1$ provides a transition, with the advection–dispersion model ($\alpha = 0.5$, blue thick dashed line) being closer to plug flow than to the gamma distribution. By comparison, the exponential distribution is closer to the gamma limit, however, in this case $\zeta = 1$. We also include the log-normal distribution for comparison (green thick dotted line), for which early arrival is bounded by TOSS with $\alpha$ in the range 0.4–0.5 (figure 2(a)). The tail part of the distributions is relatively compact (figure 2(b)), apart from the plug flow ($\alpha = 1$, black dotted line) and the anomalous case ($\alpha = 1/2$ and $\alpha = 0$, orange dotted line).

Finally, the case of extreme dispersion with $\zeta = 100$ is illustrated in figure 3 with emphasis on the tail part of the distributions. Clearly, a power-law tail is maintained for a large interval of $\theta$ until a gradual convergence to a step function is observed for $\alpha \rightarrow 1$ (figure 3). The tail cut-off is seen

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**Figure 1.** Dependence of dimensionless TOSS density parameters on the coefficient of variation $\zeta$ and exponent $\alpha$: (a) parameter $a\bar{\tau} = (1 - \alpha)/\zeta^2$, and (b) parameter $c/\bar{\tau}^\alpha = \zeta^{2\alpha-1}(1 - \alpha)^{1-\alpha}/\alpha$. The exponent $\alpha$ changes in intervals of 0.1. The colored curves are computed as the limiting cases given in table A.1.
Figure 2. Distributions of normalized WRT $\theta = \tau / \bar{\tau}$ using the TOSS density with different values of the exponent $\alpha$, including limiting cases (table A.1), for $\xi = 1.2$: (a) cumulative distribution function; (b) complementary cumulative distribution function. The exponent $\alpha$ changes in intervals of 0.1.

around $\theta = 10,000$ which corresponds to the cut-off rate of roughly $a = 10^{-4}$ (figure 1(a)); the one-sided stable density ($a \to 0$, $\alpha = 1/2$, orange thick dotted curve) maintains the tail indefinitely. Interestingly, the tail of the log-normal distribution for such a large dispersion cannot be reproduced with the TOSS density (green dotted curve, figure 3).

5. Discussion

The power-law tails associated with non-Gaussian stable distributions have been found to be useful for describing highly variable phenomena of relevance to environmental applications [7, 28, 30, 39, 32, 34]. However physical considerations and careful analyses of large-data sets (e.g. [31]) reveal that it is often necessary to modify stochastic models based on stable distributions to tame the wild variability inherent in those models. Mantegna and Stanley [23, 24] introduced a truncated or tempered version of the symmetric stable distribution, which has found wide applications in finance modeling [3, 4] as well as in the analysis of diffusion processes [1, 28]. The asymmetric (or ‘one-sided’) form of the tempered stable distribution $\tilde{\psi}(1)$ or $\tilde{f}(\tau)$ (3) was first proposed in [7] as a truncation of the asymmetric (one-sided) stable (Levy) density for tracer transport in groundwater. A general mathematical framework that unifies both the symmetric and asymmetric tempered stable distributions was developed by Rosinski [38] where the form (3) is deduced as a special case for a one-dimensional, non-negative random process (example 2, p 688).

Figure 3. The complementary cumulative distribution function of normalized WRT $\theta = \tau / \bar{\tau}$ using the TOSS density with different values of the exponent $\alpha$, including limiting cases (table A.1), for $\xi = 100$. The exponent $\alpha$ changes in intervals of 0.1.

Environmental applications of hydrological transport processes can be very different, in terms of media properties and structure, as well as in terms of temporal and spatial scales. Hence there is a need for statistical models that are sufficiently general but are relatively simple to implement, e.g. in risk assessment or interpretation of field experiments. One important class of applications is related to the geological disposal of nuclear waste in granitic rock where risk assessment is based on following hydrological transport from a hypothetical canister leak, through the filling material of the repository tunnels, the complex discrete fracture network system, the granular media of the overburden, and finally to the unsaturated soil or the sediment of the biosphere. Such a transport pathway of a passive tracer (water particle) extends over hundreds of meters and over several years, through multiple heterogeneous subsystems. The TOSS density may then be defined for each subsystem and convoluted to yield the water residence time for the entire system that can capture possible non-Fickian dispersion in a relatively simple manner using $\tilde{\psi}(1)$ and/or $\tilde{f}(\tau)$ (3) with $(0 < \alpha < 1)$.

6. Conclusions

Water transport in hydrological systems is ultimately controlled by the hydrodynamics. Combing analytical methods with numerical simulations and field data can certainly improve our understanding of water transport, however, given the complexity of boundary conditions and internal structure on a wide range of scales, a statistical distribution of water residence times is an important modeling tool. It has been shown here that the tempered one-sided stable density is currently the most general statistical distribution for hydrological transport. The TOSS density broadens the statistical toolbox and opens new possibilities for the interpretation of data from simulations and field observations [40, 21, 13, 11, 2]. The fact that the TOSS density has a simple expression in the LT domain is a particular advantage enabling efficient computations of tracer transport subject to kinetically controlled mass transfer [7].

The most important property of the TOSS density is that it is infinitely divisible (stable) under conditions $c = \sum c_i$ and
arithmetic mean and \( \zeta \) was noted in [7], with the inverse-Gaussian in [7, 38], and with the one-sided stable density in [7].

The TOSS density for segments (1) can still be convoluted; however, in the trajectory WRT would not retain stability. The TOSS parameter \( c \) is the longitudinal distance. The equivalence with the delta function was noted in [7], with the inverse-Gaussian in [7, 38], and with the one-sided stable density in [7].

\[ a = a_i, \] which means that the model is applicable on any scale.\(^1\)

Stability ensures a seamless transition between a segment-based approach to transport as a time-domain random walk formulation [33], and an integrated trajectory formulation [8]. This is based on the assumption of statistical stationarity which also implies linearity in the \( \tau \) moments \( \bar{\tau} \) and \( \text{Var} [\tau] \) (or the TOSS parameter \( c \)) with distance. Even complex and strong heterogeneity has been shown to retain this linearity if the random heterogeneity is statistically stationary [16]. In some cases, however, non-stationarity may be important, for instance in the form of fractal scaling [29]. The segment cut-off rate \( a_i \) will then depend on the scale and the TOSS density for the trajectory WRT would not retain stability. The TOSS density for segments (1) can still be convoluted; however, in this case \( \Delta \tau \) and \( \text{Var} [\Delta \tau] \) (or \( a_i \) and \( c_i \)) would be functions of distance, consistent, for example, with an assumed fractal scaling model [29]. Exploring properties of the TOSS density for statistically non-stationary conditions is a topic for future research.

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### Appendix. Moments of the gamma and TOSS densities

The \( m \)th moment \( M(m) \) of the gamma density is computed as

\[ M(m) = \lim_{s \to 0, a \to 0} \left\{ (-1)^m \frac{d^m}{ds^m} \exp[c \ a^\alpha - c \ (a + s)^\alpha] \right\} = M(m) \]  

\[ a = \frac{1 - a_i}{\bar{\tau} \zeta} \; \quad \; c = \frac{\bar{\tau}}{a a_i^{-1}} \; \quad \; \beta = \frac{1}{\zeta^2} \]

and \( M(m) \) is given in (A.1).

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\(1\) This property allows the development of diffusion models, since any infinitely divisible law has an associated differential operator [1].
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