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Record setting during dispersive transport in porous media

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[1] How often does a contaminant 'particle' migrating in a porous medium set a distance record, i.e., advance farther from the origin than at all previous time steps? This question is of fundamental importance in characterizing the nature of the leading edge of a contaminant plume as it is transported through an aquifer. It was proven theoretically by Majumdar and Ziff (2008) that, in the 1d case for pure diffusion, record setting of a random walker scales with $n^{1/2}$, where n is the number of steps, regardless of the length and time distribution of steps. Here, we use numerical simulations, benchmarked against the 1d analytical solution, to extend this result also for pure diffusion in 2d and 3d domains. We then consider transport in the presence of a drift (i.e., advective-dispersive transport), and show that the record-setting pace of random walkers changes abruptly from $\propto n^{1/2}$ to $\propto n^1$. We explore the dependence of the prefactor on the distribution of step length and number of spatial dimensions. The key implication is that when, after a brief transitional period, the scaling regime commences, the maximum distance reached by the leading edge of a migrating contaminant plume scales linearly with n, regardless of the drift magnitude. **Citation:** Edery, Y., A. Kostinski, and B. Berkowitz (2011), Record setting during dispersive transport in porous media, *Geophys. Res. Lett.*, *38*, L16403, doi:10.1029/2011GL048558.

1. Introduction

1.1. Random Walks for Contaminant Transport

[2] Modelling contaminant transport in porous and fractured media remains a subject of intense investigation, particularly in the fields of hydrology and petroleum engineering. Considering a point source of contamination, e.g., release of a contaminant from a waste disposal site or a well, the main focus is on determining the evolution of the contaminant plume, and estimating concentration breakthrough curves at various distances. More specific questions deal with determination of first arrival times [e.g., *Nelson*, 1978], travel time distributions [e.g., *Visser et al.*, 2009], maximum travel distances [e.g., *Hudak*, 2002], and maximum transport rate [e.g., *Nimmo*, 2007].

[3] In this context, the use of random walk particle tracking methods to investigate contaminant transport in porous and fractured media is well known in a rich and extensive literature, using both Fickian (advection-dispersion equation) and non-Fickian (continuous time random walk) transport equations [e.g., *Prickett et al.*, 1981; *Kinzelbach*, 1988; *Berkowitz and Scher*, 1996; *Dentz et al.*, 2004; *Delay et al.*, 2005; *Rhodes and Blunt*, 2006; *Edery et al.*, 2010]. Here, we approach analysis of "first contaminant arrivals" from a different perspective, namely, consideration of "records" as a means to characterize maximum distances travelled by contaminant particles; this is feasible in practice as field measurement detection limits have become increasingly sensitive.

1.2. Records

[4] To provide some definitions and background on "records", consider the following. The i-th entry in a series, x_i, is a record-breaking event (record, for short) if it exceeds all previous values in the sequence. In other words, x_i is a record if $x_i > \max(x_1, x_2, \ldots x_{i-1})$. An outstanding result is that for a stationary time series of independent and identically distributed random variables (i.i.d.), the probability for the n-th entry to be a record, $p = p(n)$, is $1/n$, because each of the n entries has an equal probability of being a record. Hence, the expected number of records, $M = M(n)$, is given by [*Foster and Stuart*, 1954]

$$M(n) = 1 + 1/2 + 1/3 \ldots + 1/n \tag{1}$$

and, by Euler's formula for harmonic series, for large n,

$$M(n) \approx \ln(n) + \gamma \tag{2}$$

where γ is Euler's constant. These results have been applied, e.g., to climatology [*Anderson and Kostinski*, 2010] and economics [*Wergen et al.*, 2011].

[5] While the case of i.i.d. series has been studied extensively, much less is known about non-stationary and/or correlated series. Yet, a great many applications belong to this class. Consider, for example, random walks and their applications in dispersive transport in porous media, as referenced above. The reader can see at once that this situation is considerably richer than the i.i.d case: the record-setting can occur at two levels, according to the length of an individual particle transition or the total distance from the origin. While the former is i.i.d. and the logarithmic pace of record setting is expected, the latter is non-stationary as the random walker advances progressively farther from the origin. Does the record-setting pace for the total distance mimic that of the "on average" diffusive behavior and scale as $n^{1/2}$? Indeed, it does. The square-root dependence wins over the logarithm.

[6] To be more precise, let us consider consecutive positions of a random walker (in any number of spatial dimensions) or absolute distances from the origin $l = l(n)$ as a non-stationary time series. *Majumdar and Ziff* [2008] showed that the probability distribution $p(M, n)$ of M records in n steps is universal, i.e., independent of the distribution of step lengths, for diffusion in one-dimensional (1d) systems. In particular, moments such as the mean record-setting pace for random walks are universal, so that the mean number of

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records $M(n)$ scales with a square root of the number of steps, $n^{1/2}$. Note, however, that in contrast to *Majumdar and Ziff* [2008], in this report we work with absolute distance (rather than position along the x-axis) as our main random variable. Aside from closer connection to experiments, this choice enables comparison to two and three dimensions (2d, 3d).

[7] To facilitate comparison to the relevant literature on time series analysis, let us imagine consecutive distances, traversed by a random walker, $l = l(n)$, plotted as a time series. This time series is not stationary. Rather, the ensemble mean distance scales as $n^{1/2}$, i.e., the trend for the mean distance from the origin is in accord with the law of diffusion. In another field, motivated by global warming, statistics of records in temperature time series with a linear trend were studied [*Franke et al.*, 2010; *Wergen and Krug*, 2010; *Wergen et al.*, 2011]. Regardless of whether or not the trend is linear or $n^{1/2}$, as in the random walk context, it is natural to ask if the record setting pace will mimic that of the average scaling. *Majumdar and Ziff* [2008] showed that the mean number of records set by random walkers M does indeed follow the scaling. *Franke et al.* [2010] worked at the level of individual probabilities of a record p_n — as opposed to the expected number of records — and sought a small correction to the $1/n$ i.i.d. record probability. In particular, *Franke et al.* [2010, equation 38, p. 12] showed that the probability of a record in the presence of a linear drift is asymptotically:

$$p(n) = \frac{1}{n} + c\frac{2\sqrt{\pi}}{e^2}\sqrt{\ln(n)^2/8\pi} \tag{3}$$

where $X_n = Y_n + cn$, Y_n is the n-th entry in the i.i.d. time series and c is a trend; see also equation 5 of *Wergen and Krug* [2010].

[8] In this study, we merge the above two lines of inquiry — i.e., the random walk perspective and the time series view — and pose a different type of scaling question when exploring contaminant transport under both pure diffusion and advective-dispersive ("drift") regimes. Hence, we ask: How often does a random walker set a distance record, i.e., advance farther from the origin than at all previous steps?

2. Methods

[9] We use a random walk approach that allows consideration of transport in both advective-dispersive and pure diffusion systems [*Dentz et al.*, 2004; *Edery et al.*, 2010]. The algorithm is equivalent to solving the standard partial differential equations describing such transport in a "generic" porous or fractured medium. Full details of the specific random walk algorithm are given by *Edery et al.* [2010].

[10] Three different transition (step) length probability density functions (pdfs) are considered for each step in the random walk, namely, constant unit length, exponential and truncated power law (TPL) (see *Edery et al.* [2010] for details). While the TPL pdf for spatial transitions (as opposed to temporal transitions) is less relevant for transport in porous media (see *Berkowitz et al.* [2006] and *Dentz et al.* [2008] for in-depth discussion), it is included here to examine the robustness of the record scaling behavior.

[11] We consider a random walk on an orthogonal lattice, with contaminant particles starting from the origin. The number of transitions is counted, rather than the time required for each transition. Simulations are carried out with 5000 particles in 1d, 2d and 3d; a sensitivity analysis is employed to ensure that the number of particles is sufficient to obtain representative statistics. In all simulations, the root mean square distance travelled by each particle from the origin, at each step, is calculated and the occurrence of a "record" (new largest distance travelled) for each particle is flagged. As mentioned above, to facilitate exploration beyond 1d, we work with the records of the root mean square distance from the origin, $l = l(n)$, rather than a 1d projection as of *Majumdar and Ziff* [2008].

[12] In the case of pure diffusion, at each step, the direction for a particle transition is chosen from a uniform distribution. For a random walk with a constant drift, representing a "generic" advective-dispersive transport, the probabilities for a particle transition in each direction are not equal. To choose a preferred direction, $\mathcal{D}_p$, defined along the positive x axis (with $\mathcal{D}_r$ a random direction other than $\mathcal{D}_p$), we first choose δ in the range [0,1]. If $0 < \delta < p(\mathcal{D}_p)$, then the particle advances in the $\mathcal{D}_p$ direction. The span of numbers from 0 to 1 is divided according to the "drift strength" $\varepsilon \in [0,1]$, where the larger part of this span belongs to $p(\mathcal{D}_r)$ and the rest is divided equally among the other directions:

$$p(\mathcal{D}_p) = \frac{1 + \epsilon(2d-1)}{2d}, \tag{4a}$$

$$p(\mathcal{D}_r) = \frac{1 - \epsilon}{2d}, \tag{4b}$$

with d the dimension. A pure diffusion random walk is recovered for $\epsilon = 0$.

3. Results and Discussion

[13] We begin by confirming and generalizing the 1d results of *Majumdar and Ziff* [2008] for a pure diffusion random walk, considering record-setting for the absolute distance from the origin. Significantly, we find that the expected number of records for the absolute distance, $M(n) \propto n^{1/2}$, not only for a 1d random walk with constant transition lengths, but also for the root mean square distance from the origin in 2d and 3d, for the three considered (constant length, exponential, TPL) transition length pdfs. Figures 1a–1c demonstrate this behavior for simulations in 3d, for the exponential and TPL length distributions; similar results, not shown here, are found also for simulations in 1d and 2d, for all three transition length pdfs. In all cases, the $n^{1/2}$ scaling behavior for $M(n)$, averaged over 5000 particles, is reached quickly, within 1000 steps. It should be noted that although all of these simulations demonstrate a similar scaling exponent of 1/2 for all of the pdfs and lattice dimensions, the scaling behavior of the absolute (root mean square) distances, r, travelled from the origin varies significantly (Figures 1d–1f). The constant and exponential pdf transition lengths yield the usual scaling behavior $r \propto n^{1/2}$.

[14] Consider next a random walk with drift, representing (for example) advective-dispersive of a contaminant in a porous medium. The following simple observation of limiting cases motivates our exploration. For a deterministic walk in a given direction, every step sets a new record, so that $M(n) = n^1$. On the other hand, n^0 scaling can also occur for the "back and forth" walker. The stationary series record-setting pace is logarithmic (see equation 2) while that of a random

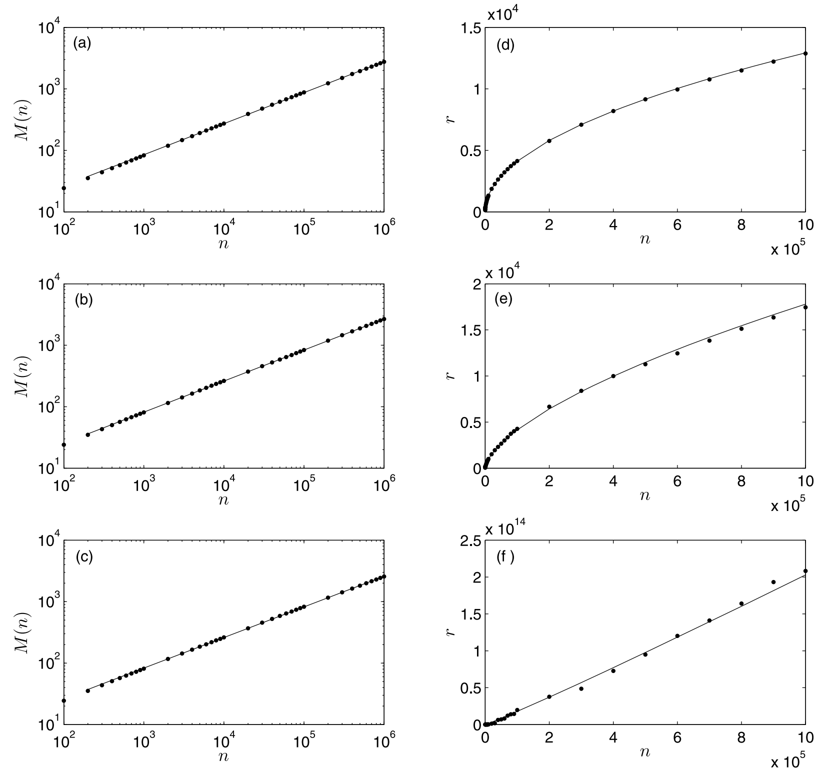

Figure 1. Random walk simulations for pure diffusion in a 3d domain, for exponential and TPL length transition pdfs, on a log-log scale. (a–c) Mean number of records, $M(n)$, versus number of steps, n (simulations: dots; lines: power law fits showing $M(n) \propto n^{1/2}$). (a): Exponential pdf, with mean = 10; (b), (c): TPL pdf with characteristic transition length = 1, cut-off length = 10^5, and $\beta = 1.6$ and 0.5, respectively. In the TPL, $0 < \beta < 2$, where $\beta \rightarrow 2$ yields Gaussian behavior, and decreasing β produces an increasingly skewed distribution with a heavy forward tail, resulting in many short length transitions and an occasional very long transition. (d–f) Root mean square distance from the origin, r, versus the number of steps, for random walk simulations corresponding to those in Figures 1a–1c, respectively. Simulations: dots; lines: power law fits showing $r \propto t^{\exp}$, where exp = 0.5, 0.63 and 1.05 for Figures 1d, 1e, and 1f, respectively.

walker is $\propto n^{1/2}$. These extremes suggest the notion of a scaling exponent. Hence, we ask: is there a range of possibilities described by the relation $M(n) \propto n^{\alpha}$, $0 \leq \alpha \leq 1$ for nonstationary series?

[15] Once posed, the question can be readily explored for random walks with a drift. Indeed, consider, for example, the simplest 1d random walk with probabilities p and $1 - p$ of a unit step in the positive and negative directions, respectively. Furthermore, let $p = 1/2 + \epsilon/2$, with $\epsilon \in [0, 1]$. Then, after n steps, the average net displacement is ϵn, so that the "drift speed" is ϵ. Hence, asymptotically, the random walker is moving in the same direction. This simple argument suggests that the record-setting pace may scale with n. Furthermore, this arguments holds for several dimensions and is independent of the distribution of steps, as is indeed confirmed by our numerical experiments, described next.

[16] Figure 2 shows results of our simulations for a random walk with drift, using the constant length spatial pdf in 1d, 2d and 3d, and for three different values of the drift value ϵ. This simple biasing of the random walk has an enormous impact on the rate of record formation. Rather remarkably, however weak the drift, α switches from 1/2 to 1 discontinuously. The number of steps required to reach the scaling regime, transitioning from 1/2 to 1, of course increases with decreasing drift strength. For $\epsilon = 0.5$ and $\epsilon = 0.1$, $\alpha = 1$ scaling is attained in less than 200 and 1000 steps, respectively, for all dimensions. For $\epsilon = 0.01$, $\alpha = 1$ scaling is attained after 20,000–30,000 steps.

[17] Furthermore, this abrupt scaling transition in the presence of drift is identical also for the exponential transition length distribution, with results similar to those shown in Figure 2. Again, for $\epsilon = 0.5$ and $\epsilon = 0.1$, $\alpha = 1$ scaling is attained in less than 200 and 1100 steps, respectively, for all dimensions. For $\epsilon = 0.01$, $\alpha = 1$ scaling is attained after 60,000–70,000 steps.

[18] Random walk simulations with drift using the TPL transition length distribution indicate a similar, but more extreme, behavior. For $\beta = 1.9$, which is relatively close to the exponential pdf, $\alpha = 1$ for all ϵ values and all three dimensions. Similar to the constant and exponential length distributions, less than 200 steps are required to reach $\alpha = 1$ scaling for $\epsilon = 0.5$, for all dimensions. However, for $\epsilon = 0.1$, 5,000–6,000 steps are required, and for $\epsilon = 0.01$, 30,000, 20,000 and 10,000 are required for, respectively, 1d, 2d and 3d. As β decreases, the transition length pdf becomes increasingly asymmetrical, with a longer tail, and the number of steps required until $\alpha = 1$ increases significantly. Thus, for example, with $\beta = 1.2$, 800 (1d) and 500 (2d, 3d) steps are required for $\epsilon = 0.5$, while for $\epsilon = 0.1$, 10,000 (1d), 7,000 (2d) and 6,000 (3d) steps are needed. For $\epsilon = 0.01$, however, $\alpha \approx$

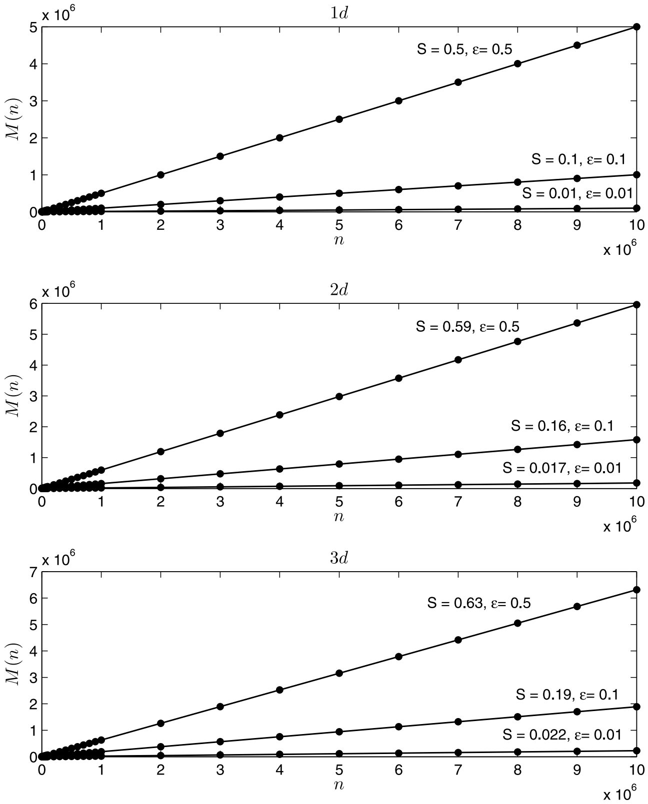

Figure 2. Mean number of records (dots) versus number of steps, on a log-log scale, for constant length transitions. The slopes (denoted S) of the linear fits correspond to the various values of ϵ.

0.53 even after ten million steps. Moreover, for $\beta = 0.5$, $\alpha < 1$ even for $\epsilon = 0.5$, after ten million steps; the cut-off in the TPL pdf guarantees that, eventually, $\alpha \rightarrow 1$. However, in practical terms for contaminant transport, the scaling behavior never reaches $\alpha = 1$ for lower β values. Note also that a time- or space-dependent drift could be considered, to account for transport in a heterogeneous domain with time- or space-varying velocity. Indeed, we carried out a similar set of simulations using a variable drift ϵ drawn from a uniform [0,1] distribution for the constant length spatial pdf; the results reported here remain valid, affecting only the number of steps required to reach asymptotic scaling.

[19] These findings also suggest questions regarding the general framework for the record-setting pace as a power law. Specifically, we have that $M(n) = Sn^{\alpha}$, where S is given in Figure 2. While asymptotically $\alpha = 1$ for a random walk with a drift, the prefactor S is not universal and depends on the relative strength of the drift, e.g., it approaches the upper bound of unity as ϵ approaches 1/2. Tables 1 and 2 show the values of the pre-factor S for the unit length and exponential transition length distributions, respectively, for 1d, 2d, and 3d systems and different values of ϵ. Note that $S = \epsilon$ in 1d, in accord with the argument given above for the "drift speed" for a simple 1d random walk. (In contrast, we find also that for the TPL pdf with, e.g., $\beta = 1.9$, $S \neq \epsilon$ for 1d; $S = 0.42$, 0.057 and 0.0037 for $\epsilon = 0.5$, 0.1 and 0.01 respectively.) We observe that the values of S decrease (essentially as a power law with decreasing exponent) with ϵ, and increase with dimension.

Table 1. Summary of Prefactor Values, S, for Unit Length Transition Distribution in Space, for 1d, 2d, 3d and Different Values of ϵ

Dimension	$\epsilon = 0.5$	$\epsilon = 0.1$	$\epsilon = 0.01$
1d	0.50	0.10	0.01
2d	0.59	0.16	0.17
3d	0.63	0.19	0.022

Table 2. Summary of Prefactor Values, S, for Exponential Length Distribution in Space, for 1d, 2d, 3d and Different Values of ϵ

Dimension	$\epsilon = 0.5$	$\epsilon = 0.1$	$\epsilon = 0.01$
1d	0.50	0.10	0.01
2d	0.57	0.13	0.014
3d	0.61	0.15	0.017

[20] It is worth noting also that the same universality holds for scaling of records when considering a random walk with memory. We find identical behavior using the following algorithm, described for 1d, 2d and 3d simulations, using the constant length pdf: if a particle transition is to the right, the probability for the particle to choose the next step to the right increases by ϵ while the probability to make a transition to the left decreases by ϵ. If the particle then advances to the left, the next preferred advance is to the left. This was noted by *Renshaw and Hendersen* [1981, p. 410] for 1d systems, who pointed out that this type of random walk is in some sense equivalent to a walk with independent increments but with a larger effective transition length.

4. Concluding Remarks

[21] We analyzed "first contaminant arrivals" in terms of "records" as a means to characterize maximum distances travelled by contaminant particles. The key implication is that the maximum distance reached by the leading edge of a migrating contaminant plume scales linearly with the number of steps, regardless of the strength of the drift. This scaling behavior can be used as an additional means to characterize the nature of the leading edge of a contaminant plume as it is transported through an aquifer. While our emphasis here is on dispersive transport in porous media, these findings are valid for all such random walks with and without drift; in other words, any system that features random walk mechanisms with and without drift can be analyzed in terms of the methods presented here.

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References

Anderson, A., and A. B. Kostinski (2010), Reversible record breaking and variability: Temperature distributions across the globe, *J. Appl. Meteorol. Climatol.*, *49*, 1681–1691.

Berkowitz, B., and H. Scher (1996), Influence of embedded fractures on contaminant diffusion in geological formations, *Geophys. Res. Lett.*, *23*, 925–928.

Berkowitz, B., A. Cortis, M. Dentz, and H. Scher (2006), Modeling non-Fickian transport in geological formations as a continuous time random walk, *Rev. Geophys.*, *44*, RG2003, doi:10.1029/2005RG000178.

Delay, F., P. Ackerer, and C. Danquigny (2005), Simulating solute transport in porous or fractured formations using random walk particle tracking: A review, *Vadose Zone J.*, *4*, 360–379, doi:10.2136/vzj2004.0125.

Dentz, M., A. Cortis, H. Scher, and B. Berkowitz (2004), Time behavior of solute transport in heterogeneous media: transition from anomalous to normal transport, *Adv. Water Resour.*, *27*(2), 155–173, doi:10.1016/j.advwatres.2003.11.002.

Dentz, M., H. Scher, D. Holder, and B. Berkowitz (2008), Transport behavior of coupled continuous-time random walks, *Phys. Rev. E*, *78*, 041110, doi:10.1103/PhysRevE.78.041110.

Edery, Y., H. Scher, and B. Berkowitz (2010), Particle tracking model of bimolecular reactive transport in porous media, *Water Resour. Res.*, *46*, W07524, doi:10.1029/2009WR009017.

Foster, F. G., and A. Stuart (1954), Distribution-free tests in time-series based on the breaking of records, *J. R. Stat. Soc., Ser. B*, *16*, 1–22.

Franke, J., G. Wergen, and J. Krug (2010), Records and sequences of records from random variables with a linear trend, *J. Stat. Mech. Theory Exp.*, P10013, doi:10.1088/1742-5468/2010/10/P10013.

Hudak, P. F. (2002), Associations between distance lags, groundwater velocities, and detection efficiencies in groundwater monitoring networks, *Environ. Monit. Assess.*, *75*, 215–221.

Kinzelbach, W. (1988), The random walk method in pollutant transport simulation, in *Groundwater Flow and Quality Modeling*, edited by E. Custodio et al., pp. 227–245, D. Reidel, Dordrecht, Netherlands.

Majumdar, S. N., and R. M. Ziff (2008), Universal record statistics of random walks and Lévy flights, *Phys. Rev. Lett.*, *101*, 050601, doi:10.1103/PhysRevLett.101.050601.

Nelson, R. W. (1978), Evaluating the environmental consequences of groundwater contamination: 2. Obtaining location/arrival time and location/outflow quantity distributions for steady flow systems, *Water Resour. Res.*, *14*, 416–428, doi:10.1029/WR014i003p00416.

Nimmo, J. R. (2007), Simple predictions of maximum transport rate in unsaturated soil and rock, *Water Resour. Res.*, *43*, W05426, doi:10.1029/2006WR005372.

Prickett, T. A., T. G. Naymik, and C. G. Lonnquist (1981), *A Random Walk Solute Transport Model for Selected Groundwater Quality Evaluations*, *Ill. State Water Surv. Bull.*, vol. 65, 103 pp., Ill. State Water Surv., Champaign.

Renshaw, E., and R. Hendersen (1981), The correlated random walk, *J. Appl. Probab.*, *186*, 403–414.

Rhodes, M. E., and M. J. Blunt (2006), An exact particle tracking algorithm for advective-dispersive transport in networks with complete mixing at nodes, *Water Resour. Res.*, *42*, W04501, doi:10.1029/2005WR004504.

Visser, A., R. Heerdink, H. P. Broers, and M. Bierkens (2009), Travel time distributions derived from particle tracking in models containing weak sinks, *Ground Water*, *47*, 237–245, doi:10.1111/j.1745-6584.2008.00542.x.

Wergen, G., and J. Krug (2010), Record-breaking temperatures reveal a warming climate, *Europhys. Lett.*, *92*, 30008, doi:10.1209/0295-5075/92/30008.

Wergen, G., M. Bogner, and J. Krug (2011), Record statistics for biased random walks, with an application to financial data, *Phys. Rev. E*, *83*, 051109, doi:10.1103/PhysRevE.83.051109.

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