Transit Time Theory is not what it used to be

Riccardo Rigon[1], Concetta D'Amato[1], and Marialaura Bancheri[2]

[1]Università di Trento
[2]Institute for Mediterranean Agricultural and Forestry systems (ISAFOM), National Research Council

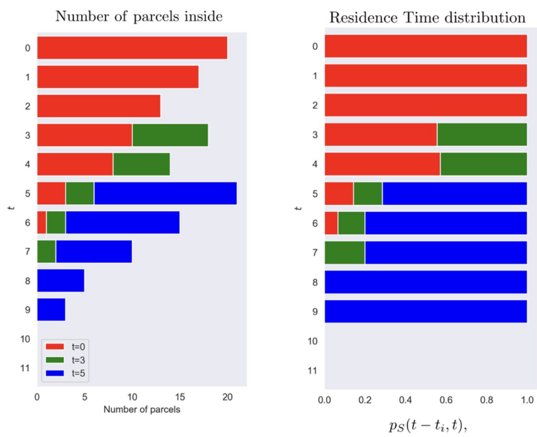
January 24, 2023

Abstract

The understating of the dynamics of tracers and water transit times at catchment scale has increasingly grown in the last decades, becoming a consolidated approach in the field of hydrological and ecohydrological research. Recently, a benchmark contribution has been given in the work by Benettin et al. (2022), which reviews the state of art on the topic, also addressing present and future challenge, pointing out some open questions in transit time research. This commentary tries to contextualize the above article, highlighting the most focal points and relating it to a broader context in the field. A brief overview on the main concepts of backward transit times, StorAge selection functions and forward transit time distributions is given in a logical-historical order, giving to the reader the primary instruments for a later comprehensive understating of the Transit Time Theory. Eventually, a numerical example helps to clarify the above concepts in a very simple and effective way.

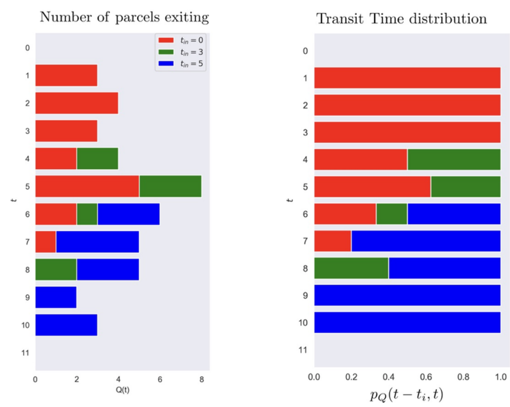
s − table

t_i →	0	3	5
t ↓			
0	20	-	-
1	17	-	-
2	13	-	-
3	10	8	-
4	8	6	-
5	3	3	15
6	1	2	12
7	0	2	8
8	-	0	5
9	-	-	3
10	-	-	0
11	-	-	-



q − table

t_i →	0	3	5
t_{ex} ↓			
0	0	-	-
1	3	-	-
2	4	-	-
3	3	0	-
4	2	2	-
5	5	3	0
6	2	1	3
7	1	0	4
8	0	2	3
9	-	0	2
10	-	-	3
11	-	-	0



Transit Time Theory is not what it used to be

Riccardo Rigon, Concetta D'Amato, Marialaura Bancheri

[1]Centro Alimenti, Agricoltura, Ambiente, Università di Trento
[2]Dipartimento di Ingegneria Civile, Ambientale e Meccanica, Università di Trento
[3]Institute for Mediterranean Agricultural and Forestry Systems (ISAFOM), National Research Council (CNR), Portici, NA, 80055, Italy

Key Points:

- Time variant Transit Time Theories (T3) are becoming more important in the hydrological studies.
- By using T3 tracer and isotope dynamics can be completely understood.
- Transit Time and Residence Time can be effectively connected by StorAge Selection functions (SAS)
- Transit Time and Residence Time distributions are connected by Niemi's identity when one is affected by celerities the other is also.

Corresponding author: Riccardo Rigon, riccardo.rigon@unitn.it

Abstract

The understanding of the dynamics of tracers and water transit times at catchment scale has increasingly grown in the last decade, becoming a consolidated approach in the field of hydrological and ecohydrological research. Recently, a benchmark contribution was made in the work by Benettin et al. (2022), which reviews the state of the art on the topic, addresses present and future challenges, and points out some open questions in transit time research. This commentary tries to contextualize the aforementioned article, highlighting its most focal points, and relating it to a broader context in the field. A brief overview of the main concepts of backward transit times, StorAge selection functions and forward transit time distributions is given in a logical-historical order, providing the reader with the primary instruments needed for a comprehensive understanding of Transit Time Theory (T3). Finally, a numerical example helps to clarify the above concepts in a very simple and effective way.

1 Introduction

Is the mathematical description of the dynamics of tracers and water *transit times* (TT) at catchment scale completely understood? The recent contribution by Benettin et al. (2022) gives a comprehensive review of the topic, which summarizes the state of the art. With T3 representing the most consistent ways to build statistical mechanics of water movements in catchments, now supported by the increasing availability of measurements made with isotopes, Benettin et al. (2022) is a timely and welcome contribution. T3 have followed two converging pathways, one coming from the works on chemical reactions and mixing of the late sixties, (e.g., Nauman, 1969), and the other crossing the history of the geomorphological instantaneous unit hydrograph, GIUH, (Rodriguez-Iturbe & Valdes, 1979; Rigon, Bancheri, Formetta, & de Lavenne, 2016). Both paths use the concept of "times distributions" but in different ways. When dealing with tracers or chemicals, we are looking at the histories of water parcels (ideal groups of water and molecules of solutes that move together across a control volume) since their injection into the control volume. Whereas when it comes to the GIUH, we are guessing what will be the hydrologic response in the future.

2 Backward transit (travel) times

Let us imagine an observer who, sitting at the outlet(s) of a control volume, records the composition of water and solute exiting the control volume at any time step and analyzes the age distribution by means of the presence of isotopes (Klaus & McDonnell, 2013). This distribution is called *backward transit time distribution* (BTTD) and has been variably indicated in literature as $\overleftarrow{p}_Q\,(T,t)$ or $p_Q(t{-}t_i|t)$ or $p_Q(T,t)$. We will use the last notation, as in Benettin et al. (2022), even though the conditional nature of these probabilities (Botter et al., 2010; Rigon, Bancheri, & Green, 2016) would suggest that the second notation is more rigorous and informative. $T := t - t_i$ is the transit time, t_i is the precipitation (injection) time, while for the observer at the outlet the current time t is the exit time, t_{ex}, by definition. In the most general case BTTD vary from time to time, i.e. they are *time-variant*, due to the complexity of the internal paths in the control volumes; this is shown in Fig. 1, where each row of the q-table identifies a different distribution. Time invariant BTTD can be caused either by a stationary velocity field or when the heterogeneity of the control volume is so high that complete randomness dominates the system (Dooge, 1986). However, stationarity is a rare case that in hydrological contexts can be altered quite simply with the injection of new water, as established by the laws of water and solute dynamics in all known media. Randomness, on the other hand, is arguably more common, especially when water flows across soil and aquifers (Dagan, 1986).

Recent studies on catchment dynamics (Durighetto & Botter, 2022) establish that catchments do indeed tend to have defined behaviours that repeat in the same way under similar forcing conditions. This suggests that transit times can vary with the intensity of precipitation and droughts but are repeated similarly in the same catchment when the same conditions are verified, as previously modelled by Godsey and Kirchner (2014). Any variation of the velocities field in the control volume must logically be attributed to hydraulic head changes that propagate pressure waves, i.e. celerities (McDonnell & Beven, 2014). Historically, given the gap between what can be theorized and what can be measured and discriminated in the field, BTTD were modelled using *time independent* transit times distributions (Maloszewski & Zuber, 1996; McGuire & McDonnell, 2006), which can be understood as an overall mean behaviour of the system through time.

A complementary approach to the one just described that uses distributions was generated in literature by categorizing the water age as "old" and "new" and analyzing their ratio. This was deemed more appropriate to the discrimination capabilities of current field surveys and measurements (Kirchner, 2019) and, given its relatively modest data requirements, has emerged as a tool to quantify the fraction of water moving through the catchment on time scales of hours, days, or weeks (Benettin et al., 2022).

3 StorAge Selection Functions

Differently from what was believed in the past, the age distribution of parcels inside the catchment, called *Backward Residence Time Distribution* (BRTD), is different from the the BTTD. This can be grasped with a simple example, (e.g., Rigon, Bancheri, & Green, 2016), illustrated in Figure 1 and comparing the BRTD toys distributions on top right with the BTTD distribution on the bottom right.

Analogously to the BTTD, the BRTD has been indicated in literature as $\overleftarrow{p}_S(T,t)$ or $p_S(t-t_i|t)$ or $p_S(T,t)$ but we will use the last notation as in Benettin et al. (2022). As shown in the pioneering work of Botter et al. (2010, 2011), the two distributions can be related through some physical-hydrological hypotheses, leading to a group of solutions for the dynamics of water. The functions relating the BTTD and the BRTD were named StorAge Selection functions (Rinaldo et al., 2015; Harman, 2015) or SAS. It can be defined as:

$$\omega_Q(T,t) := \frac{p_Q(T,t)}{p_S(T,t)} \tag{1}$$

where ':=' means "is defined as", $\omega_Q(T,t)$ is the notation for SAS and the probabilities on the right-hand side were defined previously. The conceptual meaning of SAS can be easily grasped considering that them correspond to the rules with which the water parcels inside a control volume are selected by hydrological dynamics to exit it; the water parcels are eventually recorded at the outlets. The simplest SAS, the identity $\omega_Q = 1$, corresponds to the uniform selection of water parcels from the population of water parcels in the control volume, without favouring a particular subset of ages. In this case BTTD and BRTD coincide and the form of the BTTD is known simply by solving the water budget (Botter et al., 2011):

$$p_Q(T,t) = \frac{J(t_i)}{S(t_i)} e^{-\int_{t-T}^{t} \frac{J(x)}{S(x)} dx} \tag{2}$$

where $J(x)$ is the precipitation input at time x and $S(x)$ is the total volume of water stored in the control volume at time x. Equation (2) is a solution that generalizes the results of Nauman (1969), which is further generalized in Botter et al. (2011). Benettin et al. (2022) provides an accurate review on how the SAS is obtained and characterized against measurements. Notably, the most recent assessment technique to obtain it is to assign the so-called cumulative SAS, $\Omega_Q(T,t)$, which is equivalent to the cumulative transit time s – table

t ↓ / t_i →	0	3	5
0	20	-	-
1	17	-	-
2	13	-	-
3	10	8	-
4	8	6	-
5	3	3	15
6	1	2	12
7	0	2	8
8	-	0	5
9	-	-	3
10	-	-	0
11	-	-	-

q – table

t_{ex} ↓ / t_i →	0	3	5
0	0	-	-
1	3	-	-
2	4	-	-
3	3	0	-
4	2	2	-
5	5	3	0
6	2	1	3
7	1	0	4
8	0	2	3
9	-	0	2
10	-	-	3
11	-	-	0

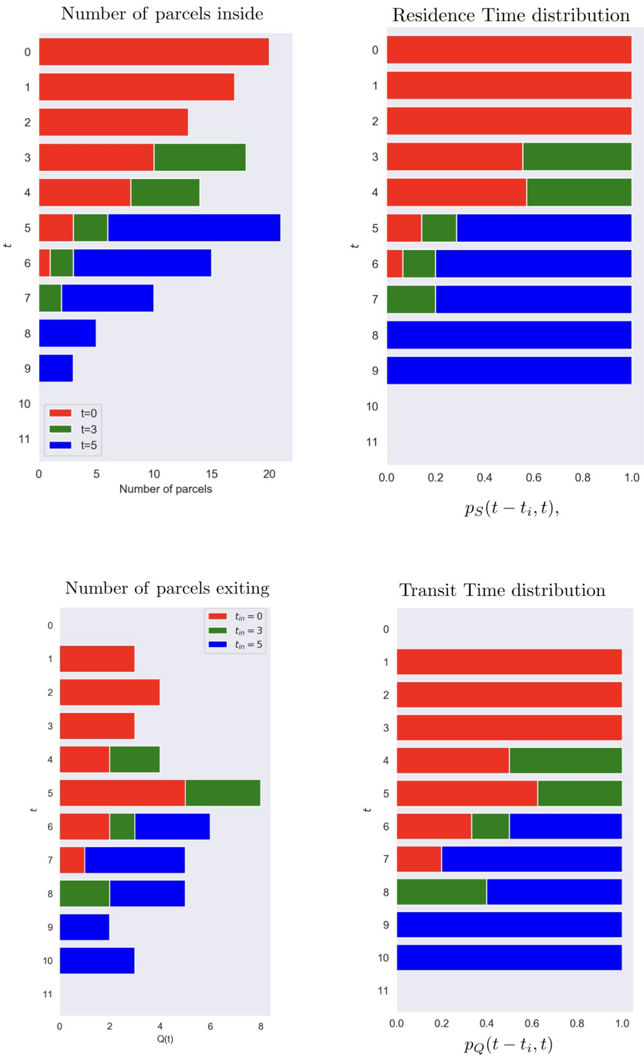


Figure 1. The figure represents the hypothetical set of water parcels of a control volume (top left table, or s-table) and the corresponding discharges (bottom left table, or q-table). The central column represents, respectively, at the top, the number of water parcels inside the control volume and, at the bottom, the number of water parcel exiting the control volume. The different colours represent rainfall injected at different injection times and, at any time t, the bars reflect the age composition of the storage (top center) and discharge (bottom center). On the right column the total number of parcels, both for resident and exiting parcels, are normalized to 1, thus representing the backward residence time probability distribution and the backward transit time probability distribution (top and bottom respectively). The Figure also reveals the discrete nature of these distributions. Further comments are in the text.

distribution function between [0,T]. That is to say:

$$\Omega_Q(T,t) := \int_{t-T}^{t} p_Q(t-t_i|t)dt_i = \int_{t-T}^{t} \omega_Q(t,t_i)p_S(t-t_i|t)dt_i = \int_{0}^{p_S(T|t)} \omega_Q(P_S,t)dP_S \quad (3)$$

Usually, $\Omega_Q(T,t)$ is written as $\Omega_Q(S_T(T,t),t)$ to highlight that the dependence of Ω_Q on t_i is mediated by a dependence on the cumulative storage S_T, defined as the total volume of storage of parcels whose age is between [0,T]. As shown in Benettin et al. (2022), the literature has provided various forms for the $\Omega_Q(T,t)$ function, which have given excellent results in analyzing field cases. Finding ways to assign Ω or related quantities is one key aspect to which Benettin et al. (2022) offers a valuable review.

A typical example of Ω, for instance, can be:

$$\Omega_Q(P_S) = P_S^k \quad (4)$$

where P_S is the probability associated with the BRTD and k is a parameter that favours the selection of young water if less than 1 and of old water if greater than 1 (Benettin et al., 2017; Harman, 2019).

4 Forward transit time distribution (a.k.a. the Hydrologic response) and Niemi's identity

It has been known since the seventies that BTTD do not coincide with the forward transit time distributions (Niemi, 1977). The latter are usually thought of as hypotheses on the life expectancy of the population of water parcels injected into a control volume at a given input time (Rigon & Bancheri, 2021) and can be identified with a generalization of the integral operator traditionally known as instantaneous unit hydrograph, $IUH(T|t_i)$, made time varying. This restricted life expectancy is, by construction, conditional on the injection, i.e., on the precipitation time. The number of IUHs is discrete and numerable, while the IUHs themselves are continuous functions of t. In Figure 1, each columns of the q-table is an IUH, normalized by the total amount of precipitation at time t_i, i.e., the first (non null) entry of the same column in the s-table. Niemi's identity thus reads:

$$IUH(T|t_i)J(t_i) \equiv p_Q(T,t_i)Q(t) \quad (5)$$

where IUH is the travel time distribution, J is the precipitation, and $Q(t)$ is the discharge. More complex expressions need to be used if the water parcels can exit the control volume in other ways, for instance as transpiration, besides as surface runoff. The identity can be misleading because it is often unclear to the reader that it cannot be used to forecast the future (i.e., the IUH) from the past (i.e., using the BTTD) unless some hypothesis of time invariance is made. This part is not explicitly treated in Benettin et al. (2022) but can be found in Rigon, Bancheri, and Green (2016) and Rigon and Bancheri (2021).

Niemi's identity is a powerful machine to extract knowledge from the past, probably as powerful as the Bayes formula, even if it has not been exploited enough so far. For any time t, in fact, all the past IUHs, each one corresponding to a different precipitation time, can be obtained and the whole sequence used to explore its variability. In principle, some water parcels can take infinite time to exit the control volume. However, in practice, after a reasonable characteristic time, only an irrelevant part of what was injected has still to exit, for example an arbitrary portion of 0.001, and can be neglected for all practical purposes. This arbitrary choice would identify, in the old parlance of IUH theory, the concentration time of a particular catchment under its specific climate history.

Niemi's identity, on the other hand, shows that if the BTTD are affected by celerity then so should the hydrologic response be.

5 The Swiss Army knife for understanding

The Swiss Army knife for understanding all of the above relationships is given by the decomposition of both the backward and forward probabilities in terms of the age-ranked discharges (van der Velde et al., 2012; Benettin et al., 2013; Harman, 2019), which are actually the functions tabulated in Figure 1. The s-table in the figure is a discrete representation of the age-ranked storage, $s(t, t_i)$, for which:

$$S(t) = \sum_{\forall t_i} s(t, t_i) \tag{6}$$

where $S(t)$ is the total water present in the control volume. The age ranked discharges, $q(t, t_i)$, are represented in the q-table and for them a relation similar to equation (6) is valid. They represent the decomposition of a given discharge according to the ages that compose it (or, which is equivalent, the precipitation time). All the details of these decomposition can be found, for instance, in Rigon, Bancheri, and Green (2016). Here we give a brief compendium based on Figure 1 where the entries of the q-table are the age-ranked discharge recorded at discrete times. If we focus just on new water and old water, these can be obtained by separating the columns of the q-table in the figure into two groups, before and after a certain date t_i (included), and the columns entries summed together.

The use of age-ranked functions not only makes Niemi's identity trivial, corresponding to the intersection of a given column (from which the IUH is obtained) and a given row (from which the BTTD is obtained) in the q-table, but also suggests easy numerical methods for the computation of any of the quantities presented in the previous descriptions.

6 Conclusions

The result of the above findings, well described in Benettin et al. (2022), is that in recent years a great number of papers have embraced the new insights for investigating how water moves in hillslopes, either using the approach shown in Kirchner (2019) or the SAS approach. Using process-based approaches, database approaches and their variations (Meira Neto et al., 2022), it has been possible to determine that transport mechanisms vary greatly between wet and dry periods, due to the interplay of surface runoff, soil flow and groundwater contribution (Soulsby et al., 2015; Tetzlaff et al., 2014; Wilusz et al., 2017; von Freyberg et al., 2017; Knapp et al., 2019). Various papers, as reported in Benettin et al. (2022), have described the mechanism of activation of flows of old water and the impact of new precipitation.

Besides, the indications derived from the new T3 approaches are also affecting the way catchments are modelled. Because it has been shown that to any model structure there corresponds a travel time signature (Rigon & Bancheri, 2021), the model-used-as-hypothesis approach (Clark et al., 2011; Beven, 2018) has acquired new tools to be exploited.

As emphasized in the last sections of Benettin et al. (2022), using T3 allows for more than just predicting discharges of water and solutes. It opens new directions for the investigation of the whole hydrological cycle (McDonnell, 2014), especially in assessing how vegetation uses water of different ages.

Eventually, these and others new challenges are carefully reviewed in Benettin et al. (2022) opening up, as Li et al. (2021) states, to the development of integrated Earth system science theories at the intersection of hydrology, biology and geochemistry, following the call for understanding of climate-soil-vegetation dynamics that started with Rodriguez-Iturbe (2000).

Acknowledgments

All the Authors contributed equally to this commentary. It was partially financed by the WATERSTEM PRIN project. A few videos were prepared to illustrate the concepts of the commentary, which can be found here: https://vimeo.com/showcase/10101034

References

Benettin, P., Rinaldo, A., & Botter, G. (2013, December). Kinematics of age mixing in advection-dispersion models. *Water Resour. Res.*, *49*(12), 8539–8551.

Benettin, P., Rodriguez, N. B., Sprenger, M., Kim, M., Klaus, J., Harman, C. J., . . . McDonnell, J. J. (2022, November). Transit time estimation in catchments: Recent developments and future directions. *Water Resour. Res.*, *58*(11).

Benettin, P., Soulsby, C., Birkel, C., Tetzlaff, D., Botter, G., & Rinaldo, A. (2017, March). Using SAS functions and high-resolution isotope data to unravel travel time distributions in headwater catchments. *Water Resour. Res.*, *53*(3), 1864–1878.

Beven, K. J. (2018, May). On hypothesis testing in hydrology: Why falsification of models is still a really good idea. *WIREs Water*, *5*(3), e1278.

Botter, G., Bertuzzo, E., & Rinaldo, A. (2010, March). Transport in the hydrologic response: Travel time distributions, soil moisture dynamics, and the old water paradox. *Water Resour. Res.*, *46*(3).

Botter, G., Bertuzzo, E., & Rinaldo, A. (2011, January). Catchment residence and travel time distributions: The master equation. *Geophys. Res. Lett.*, *38*(11).

Clark, M. P., Kavetski, D., & Fenicia, F. (2011, September). Pursuing the method of multiple working hypotheses for hydrological modeling. *Water Resour. Res.*, *47*(9).

Dagan, G. (1986, September). Statistical theory of groundwater flow and transport' pore to laboratory, laboratory to formation, and formation to regional scal. *Water Resour. Res.*, *22*(9), 120–134.

Dooge, J. C. I. (1986, August). Looking for hydrologic laws. *Water Resour. Res.*, *22*(9S), 46S–58S.

Durighetto, N., & Botter, G. (2022, July). On the relation between active network length and catchment discharge. *Geophys. Res. Lett.*, *49*(14), e2022GL099500.

Godsey, S. E., & Kirchner, J. W. (2014, November). Dynamic, discontinuous stream networks: hydrologically driven variations in active drainage density, flowing channels and stream order. *Hydrol. Process.*, *28*(23), 5791–5803.

Harman, C. J. (2015, January). Time-variable transit time distributions and transport: Theory and application to storage-dependent transport of chloride in a watershed. *Water Resour. Res.*, *51*(1), 1–30.

Harman, C. J. (2019, August). Age-ranked storage-discharge relations: A unified description of spatially lumped flow and water age in hydrologic systems. *Water Resour. Res.*, *55*(8), 7143–7165.

Kirchner, J. W. (2019, January). Quantifying new water fractions and transit time distributions using ensemble hydrograph separation: theory and benchmark tests. *HESS*, *23*, 303–349.

Klaus, J., & McDonnell, J. J. (2013, November). Hydrograph separation using stable isotopes: Review and evaluation. *J. Hydrol.*, *505*(C), 47–64.

Knapp, J. L. A., Neal, C., Schlumpf, A., Neal, M., & Kirchner, J. W. (2019, June). New water fractions and transit time distributions at plynlimon, wales, estimated from stable water isotopes in precipitation and streamflow. *Hydrol. Earth Syst. Sci. Discuss.*, 1–40.

Li, L., Sullivan, P. L., Benettin, P., Cirpka, O. A., Bishop, K., Brantley, S. L., . . . Kirchner, J. W. (2021, January). Toward catchment hydro-biogeochemical theories. *WIREs Water*, *8*(1).

Maloszewski, P., & Zuber, A. (1996, October). *Lumped parameter models for the interpretation of environmental tracer data* (Tech. Rep.).

McDonnell, J. J. (2014, April). The two water worlds hypothesis: ecohydrological separation of water between streams and trees? *Wiley Interdisciplinary Reviews: Water*.

McDonnell, J. J., & Beven, K. (2014, June). Debates-The future of hydrological sciences: A (common) path forward? a call to action aimed at understanding velocities, celerities and residence time distributions of the headwater hydrograph. *Water Resour. Res.*, *50*(6), 5342–5350.

McGuire, K. J., & McDonnell, J. J. (2006, November). A review and evaluation of catchment transit time modeling. *J. Hydrol.*, *330*(3), 543–563.

Meira Neto, A. A., Kim, M., & Troch, P. A. (2022, February). Physical interpretation of time-varying StorAge selection functions in a bench-scale hillslope experiment via geophysical imaging of ages of water. *Water Resour. Res.*.

Nauman, E. B. (1969, June). Residence time distribution theory for unsteady stirred tank reactors. *Chem. Eng. Sci.*, *24*, 1471–1480.

Niemi, A. J. (1977, October). Residence time distributions of variable flow processes. *Int. J. Appl. Radiat. Isot.*, *28*(10), 855–860.

Rigon, R., & Bancheri, M. (2021, January). On the relations between the hydrological dynamical systems of water budget, travel time, response time and tracer concentrations. *Hydrol. Process.*, *35*(1).

Rigon, R., Bancheri, M., Formetta, G., & de Lavenne, A. (2016, January). The geomorphological unit hydrograph from a historical-critical perspective. *Earth Surf. Processes Landforms*, *41*(1), 27–37.

Rigon, R., Bancheri, M., & Green, T. R. (2016, May). Age-ranked hydrological budgets and a travel time description of catchment hydrology. *Hydrol. Earth Syst. Sci. Discuss.*, 1–22.

Rinaldo, A., Benettin, P., Harman, C. J., Hrachowitz, M., McGuire, K. J., van der Velde, Y., . . . Botter, G. (2015, June). Storage selection functions: A coherent framework for quantifying how catchments store and release water and solutes. *Water Resour. Res.*, *51*(6), 4840–4847.

Rodriguez-Iturbe, I. (2000). Ecohydrology: A hydrologic perspective of climate-soil-vegetation dynamics. *Water Resources Research*, *36*(1).

Rodriguez-Iturbe, I., & Valdes, J. B. (1979). The geomorphologic structure of the hydrologic response. *Water Resources Reesearch*, *15*(6), 1409–1420.

Soulsby, C., Birkel, C., Geris, J., Dick, J., Tunaley, C., & Tetzlaff, D. (2015, September). Stream water age distributions controlled by storage dynamics and nonlinear hydrologic connectivity: Modeling with high-resolution isotope data. *Water Resour. Res.*, *51*(9), 7759–7776.

Tetzlaff, D., Buttle, J., Carey, S. K., McGuire, K., Laudon, H., & Soulsby, C. (2014, December). Tracer-based assessment of flow paths, storage and runoff generation in northern catchments: a review. *Hydrol. Process.*, *29*(16), 3475–3490.

van der Velde, Y., Torfs, P. J. J. F., Van der Zee, S. E. A. T. M., & Uijlenhoet, R. (2012, June). Quantifying catchment-scale mixing and its effect on time-varying travel time distributions. *Water Resour. Res.*, *48*(6), W06536–13.

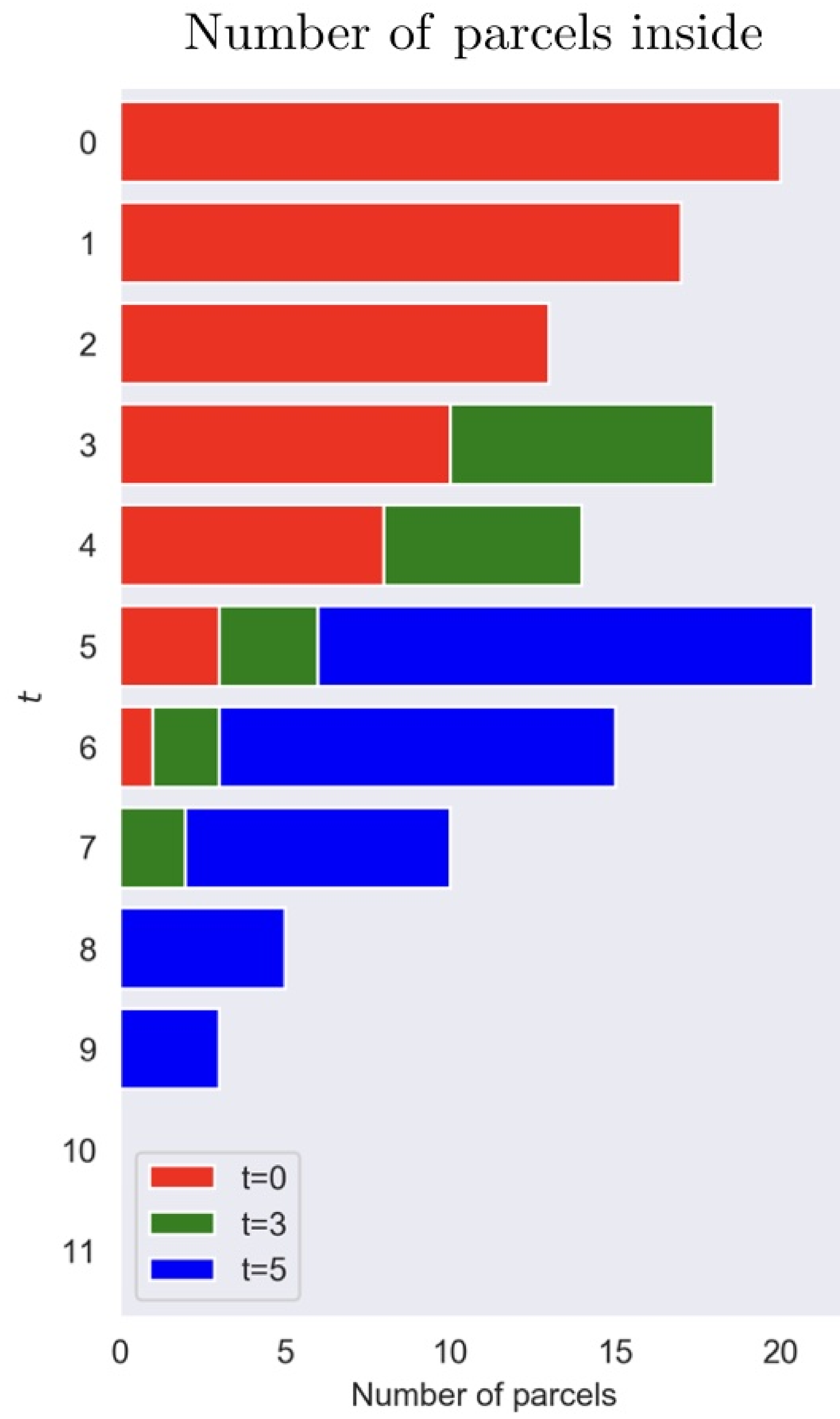
von Freyberg, J., Studer, B., & Kirchner, J. W. (2017, March). A lab in the field: high-frequency analysis of water quality and stable isotopes in stream water and precipitation. *Hydrol. Earth Syst. Sci.*, *21*(3), 1721–1739.

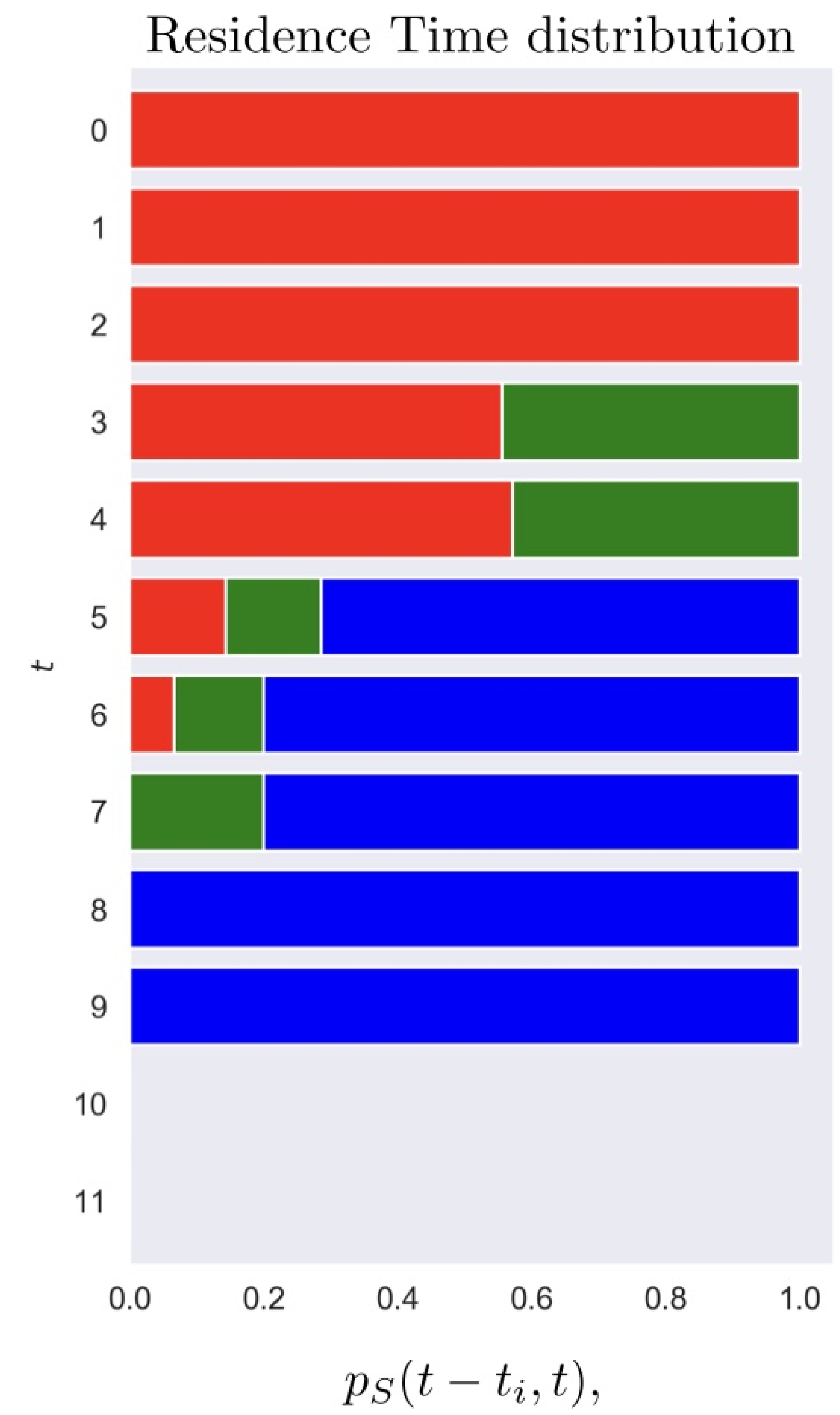
Wilusz, D. C., Harman, C. J., & Ball, W. P. (2017, December). Sensitivity of catchment transit times to rainfall variability under present and future climates. *Water Resour. Res.*, *53*(12), 10231–10256.

Figure.

s − table

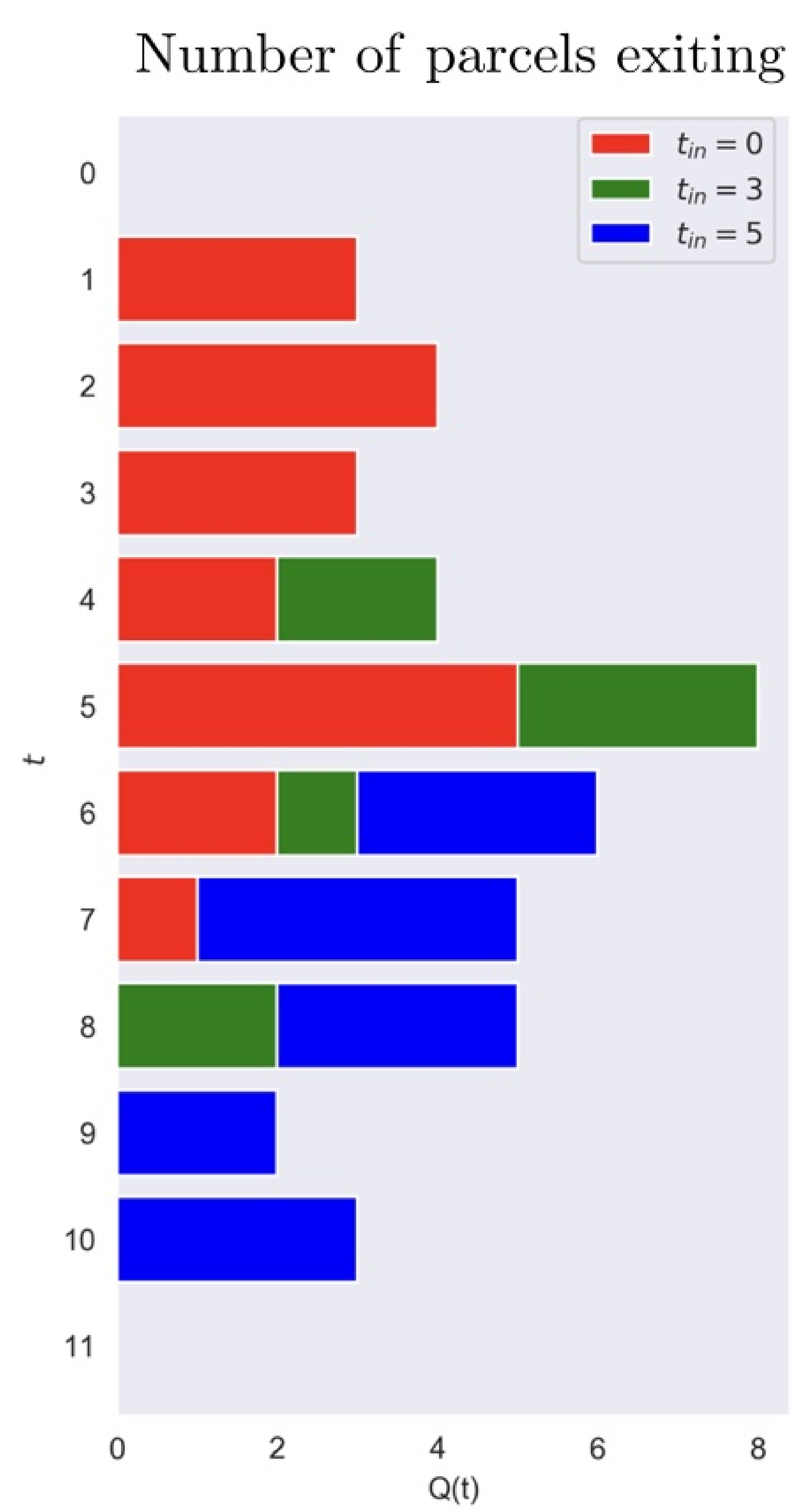
t_i →	0	3	5
t ↓			
0	20	-	-
1	17	-	-
2	13	-	-
3	10	8	-
4	8	6	-
5	3	3	15
6	1	2	12
7	0	2	8
8	-	0	5
9	-	-	3
10	-	-	0
11	-	-	-

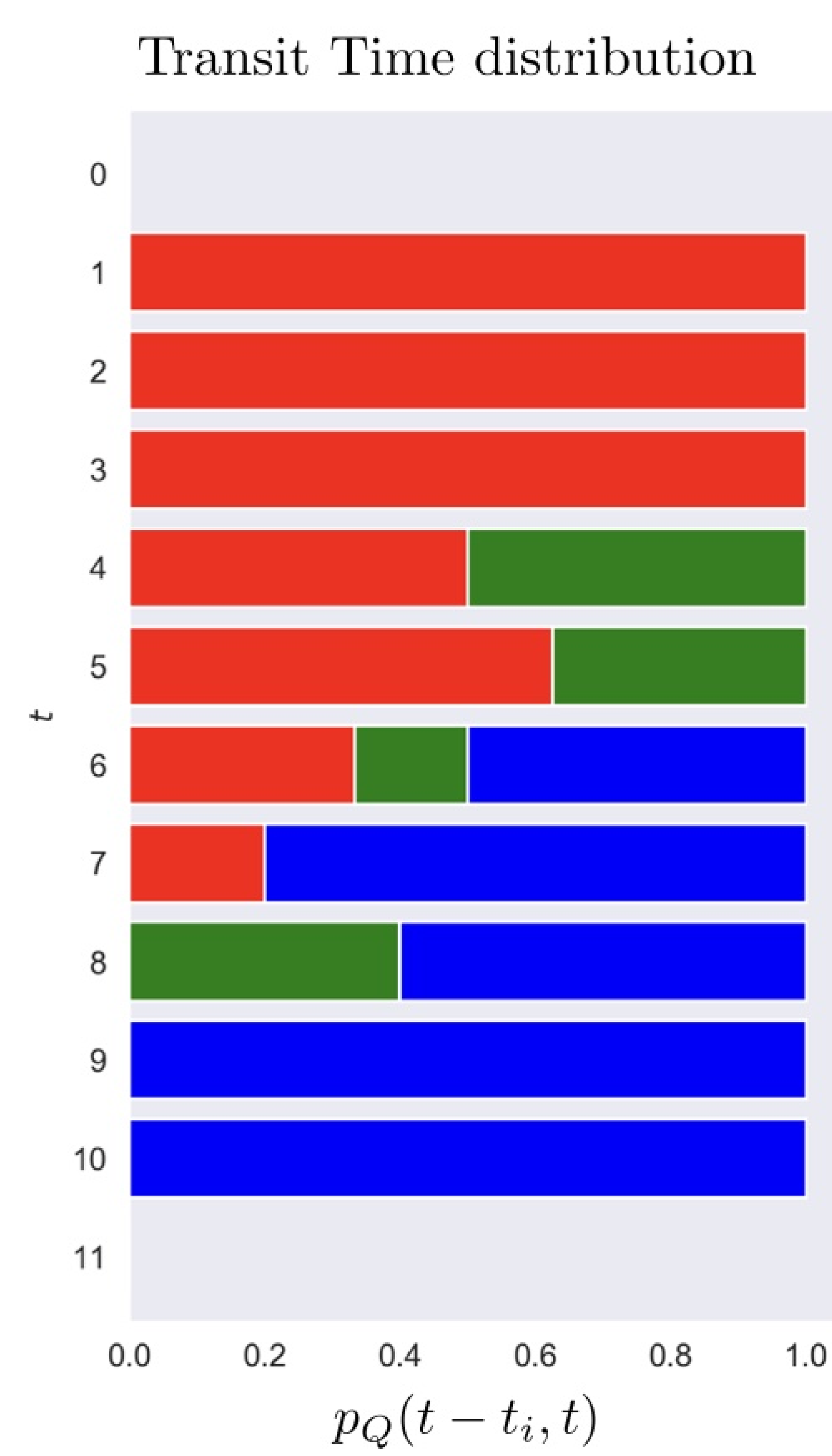




q − table

t_i →	0	3	5
t_{ex} ↓			
0	0	-	-
1	3	-	-
2	4	-	-
3	3	0	-
4	2	2	-
5	5	3	0
6	2	1	3
7	1	0	4
8	0	2	3
9	-	0	2
10	-	-	3
11	-	-	0





Transit Time Theory is not what it used to be

Riccardo Rigon, Concetta D'Amato, Marialaura Bancheri

[1]Centro Alimenti, Agricoltura, Ambiente, Università di Trento
[2]Dipartimento di Ingegneria Civile, Ambientale e Meccanica, Università di Trento
[3]Institute for Mediterranean Agricultural and Forestry Systems (ISAFOM), National Research Council (CNR), Portici, NA, 80055, Italy

Key Points:

- Time variant Transit Time Theories (T3) are becoming more important in the hydrological studies.
- By using T3 tracer and isotope dynamics can be completely understood.
- Transit Time and Residence Time can be effectively connected by StorAge Selection functions (SAS)
- Transit Time and Residence Time distributions are connected by Niemi's identity when one is affected by celerities the other is also.

Corresponding author: Riccardo Rigon, `riccardo.rigon@unitn.it`

Abstract

The understanding of the dynamics of tracers and water transit times at catchment scale has increasingly grown in the last decade, becoming a consolidated approach in the field of hydrological and ecohydrological research. Recently, a benchmark contribution was made in the work by Benettin et al. (2022), which reviews the state of the art on the topic, addresses present and future challenges, and points out some open questions in transit time research. This commentary tries to contextualize the aforementioned article, highlighting its most focal points, and relating it to a broader context in the field. A brief overview of the main concepts of backward transit times, StorAge selection functions and forward transit time distributions is given in a logical-historical order, providing the reader with the primary instruments needed for a comprehensive understanding of Transit Time Theory (T3). Finally, a numerical example helps to clarify the above concepts in a very simple and effective way.

1 Introduction

Is the mathematical description of the dynamics of tracers and water *transit times* (TT) at catchment scale completely understood? The recent contribution by Benettin et al. (2022) gives a comprehensive review of the topic, which summarizes the state of the art. With T3 representing the most consistent ways to build statistical mechanics of water movements in catchments, now supported by the increasing availability of measurements made with isotopes, Benettin et al. (2022) is a timely and welcome contribution. T3 have followed two converging pathways, one coming from the works on chemical reactions and mixing of the late sixties, (e.g., Nauman, 1969), and the other crossing the history of the geomorphological instantaneous unit hydrograph, GIUH, (Rodriguez-Iturbe & Valdes, 1979; Rigon, Bancheri, Formetta, & de Lavenne, 2016). Both paths use the concept of "times distributions" but in different ways. When dealing with tracers or chemicals, we are looking at the histories of water parcels (ideal groups of water and molecules of solutes that move together across a control volume) since their injection into the control volume. Whereas when it comes to the GIUH, we are guessing what will be the hydrologic response in the future.

2 Backward transit (travel) times

Let us imagine an observer who, sitting at the outlet(s) of a control volume, records the composition of water and solute exiting the control volume at any time step and analyzes the age distribution by means of the presence of isotopes (Klaus & McDonnell, 2013). This distribution is called *backward transit time distribution* (BTTD) and has been variably indicated in literature as $\overleftarrow{p}_Q\,(T,t)$ or $p_Q(t{-}t_i|t)$ or $p_Q(T,t)$. We will use the last notation, as in Benettin et al. (2022), even though the conditional nature of these probabilities (Botter et al., 2010; Rigon, Bancheri, & Green, 2016) would suggest that the second notation is more rigorous and informative. $T := t - t_i$ is the transit time, t_i is the precipitation (injection) time, while for the observer at the outlet the current time t is the exit time, t_{ex}, by definition. In the most general case BTTD vary from time to time, i.e. they are *time-variant*, due to the complexity of the internal paths in the control volumes; this is shown in Fig. 1, where each row of the q-table identifies a different distribution. Time invariant BTTD can be caused either by a stationary velocity field or when the heterogeneity of the control volume is so high that complete randomness dominates the system (Dooge, 1986). However, stationarity is a rare case that in hydrological contexts can be altered quite simply with the injection of new water, as established by the laws of water and solute dynamics in all known media. Randomness, on the other hand, is arguably more common, especially when water flows across soil and aquifers (Dagan, 1986).

Recent studies on catchment dynamics (Durighetto & Botter, 2022) establish that catchments do indeed tend to have defined behaviours that repeat in the same way under similar forcing conditions. This suggests that transit times can vary with the intensity of precipitation and droughts but are repeated similarly in the same catchment when the same conditions are verified, as previously modelled by Godsey and Kirchner (2014). Any variation of the velocities field in the control volume must logically be attributed to hydraulic head changes that propagate pressure waves, i.e. celerities (McDonnell & Beven, 2014). Historically, given the gap between what can be theorized and what can be measured and discriminated in the field, BTTD were modelled using *time independent* transit times distributions (Maloszewski & Zuber, 1996; McGuire & McDonnell, 2006), which can be understood as an overall mean behaviour of the system through time.

A complementary approach to the one just described that uses distributions was generated in literature by categorizing the water age as “old” and “new” and analyzing their ratio. This was deemed more appropriate to the discrimination capabilities of current field surveys and measurements (Kirchner, 2019) and, given its relatively modest data requirements, has emerged as a tool to quantify the fraction of water moving through the catchment on time scales of hours, days, or weeks (Benettin et al., 2022).

3 StorAge Selection Functions

Differently from what was believed in the past, the age distribution of parcels inside the catchment, called *Backward Residence Time Distribution* (BRTD), is different from the the BTTD. This can be grasped with a simple example, (e.g., Rigon, Bancheri, & Green, 2016), illustrated in Figure 1 and comparing the BRTD toys distributions on top right with the BTTD distribution on the bottom right.

Analogously to the BTTD, the BRTD has been indicated in literature as $\overleftarrow{p}_S\,(T,t)$ or $p_S(t{-}t_i|t)$ or $p_S(T,t)$ but we will use the last notation as in Benettin et al. (2022). As shown in the pioneering work of Botter et al. (2010, 2011), the two distributions can be related through some physical-hydrological hypotheses, leading to a group of solutions for the dynamics of water. The functions relating the BTTD and the BRTD were named StorAge Selection functions (Rinaldo et al., 2015; Harman, 2015) or SAS. It can be defined as:

$$\omega_Q(T,t) := \frac{p_Q(T,t)}{p_S(T,t)} \tag{1}$$

where ':=' means “is defined as”, $\omega_Q(T,t)$ is the notation for SAS and the probabilities on the right-hand side were defined previously. The conceptual meaning of SAS can be easily grasped considering that them correspond to the rules with which the water parcels inside a control volume are selected by hydrological dynamics to exit it; the water parcels are eventually recorded at the outlets. The simplest SAS, the identity $\omega_Q = 1$, corresponds to the uniform selection of water parcels from the population of water parcels in the control volume, without favouring a particular subset of ages. In this case BTTD and BRTD coincide and the form of the BTTD is known simply by solving the water budget (Botter et al., 2011):

$$p_Q(T,t) = \frac{J(t_i)}{S(t_i)} e^{-\int_{t-T}^{t} \frac{J(x)}{S(x)} dx} \tag{2}$$

where $J(x)$ is the precipitation input at time x and $S(x)$ is the total volume of water stored in the control volume at time x. Equation (2) is a solution that generalizes the results of Nauman (1969), which is further generalized in Botter et al. (2011). Benettin et al. (2022) provides an accurate review on how the SAS is obtained and characterized against measurements. Notably, the most recent assessment technique to obtain it is to assign the so-called cumulative SAS, $\Omega_Q(T,t)$, which is equivalent to the cumulative transit time

s − table

t ↓ / t_i →	0	3	5
0	20	-	-
1	17	-	-
2	13	-	-
3	10	8	-
4	8	6	-
5	3	3	15
6	1	2	12
7	0	2	8
8	-	0	5
9	-	-	3
10	-	-	0
11	-	-	-

q − table

t_{ex} ↓ / t_i →	0	3	5
0	0	-	-
1	3	-	-
2	4	-	-
3	3	0	-
4	2	2	-
5	5	3	0
6	2	1	3
7	1	0	4
8	0	2	3
9	-	0	2
10	-	-	3
11	-	-	0

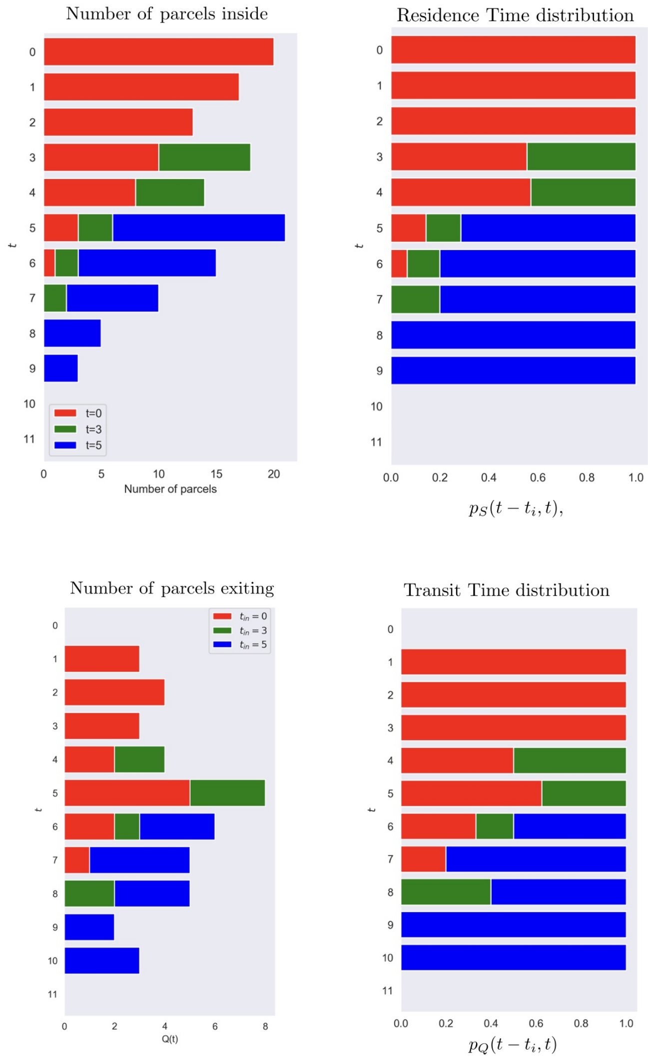


Figure 1. The figure represents the hypothetical set of water parcels of a control volume (top left table, or s-table) and the corresponding discharges (bottom left table, or q-table). The central column represents, respectively, at the top, the number of water parcels inside the control volume and, at the bottom, the number of water parcel exiting the control volume. The different colours represent rainfall injected at different injection times and, at any time t, the bars reflect the age composition of the storage (top center) and discharge (bottom center). On the right column the total number of parcels, both for resident and exiting parcels, are normalized to 1, thus representing the backward residence time probability distribution and the backward transit time probability distribution (top and bottom respectively). The Figure also reveals the discrete nature of these distributions. Further comments are in the text.

distribution function between [0,T]. That is to say:

$$\Omega_Q(T,t) := \int_{t-T}^{t} p_Q(t-t_i|t)dt_i = \int_{t-T}^{t} \omega_Q(t,t_i)p_S(t-t_i|t)dt_i = \int_0^{p_S(T|t)} \omega_Q(P_S,t)dP_S \quad (3)$$

Usually, $\Omega_Q(T,t)$ is written as $\Omega_Q(S_T(T,t),t)$ to highlight that the dependence of Ω_Q on t_i is mediated by a dependence on the cumulative storage S_T, defined as the total volume of storage of parcels whose age is between [0,T]. As shown in Benettin et al. (2022), the literature has provided various forms for the $\Omega_Q(T,t)$ function, which have given excellent results in analyzing field cases. Finding ways to assign Ω or related quantities is one key aspect to which Benettin et al. (2022) offers a valuable review.

A typical example of Ω, for instance, can be:

$$\Omega_Q(P_S) = P_S^k \quad (4)$$

where P_S is the probability associated with the BRTD and k is a parameter that favours the selection of young water if less than 1 and of old water if greater than 1 (Benettin et al., 2017; Harman, 2019).

4 Forward transit time distribution (a.k.a. the Hydrologic response) and Niemi's identity

It has been known since the seventies that BTTD do not coincide with the forward transit time distributions (Niemi, 1977). The latter are usually thought of as hypotheses on the life expectancy of the population of water parcels injected into a control volume at a given input time (Rigon & Bancheri, 2021) and can be identified with a generalization of the integral operator traditionally known as instantaneous unit hydrograph, $IUH(T|t_i)$, made time varying. This restricted life expectancy is, by construction, conditional on the injection, i.e., on the precipitation time. The number of IUHs is discrete and numerable, while the IUHs themselves are continuous functions of t. In Figure 1, each columns of the q-table is an IUH, normalized by the total amount of precipitation at time t_i, i.e., the first (non null) entry of the same column in the s-table. Niemi's identity thus reads:

$$IUH(T|t_i)J(t_i) \equiv p_Q(T,t_i)Q(t) \quad (5)$$

where IUH is the travel time distribution, J is the precipitation, and $Q(t)$ is the discharge. More complex expressions need to be used if the water parcels can exit the control volume in other ways, for instance as transpiration, besides as surface runoff. The identity can be misleading because it is often unclear to the reader that it cannot be used to forecast the future (i.e., the IUH) from the past (i.e., using the BTTD) unless some hypothesis of time invariance is made. This part is not explicitly treated in Benettin et al. (2022) but can be found in Rigon, Bancheri, and Green (2016) and Rigon and Bancheri (2021).

Niemi's identity is a powerful machine to extract knowledge from the past, probably as powerful as the Bayes formula, even if it has not been exploited enough so far. For any time t, in fact, all the past IUHs, each one corresponding to a different precipitation time, can be obtained and the whole sequence used to explore its variability. In principle, some water parcels can take infinite time to exit the control volume. However, in practice, after a reasonable characteristic time, only an irrelevant part of what was injected has still to exit, for example an arbitrary portion of 0.001, and can be neglected for all practical purposes. This arbitrary choice would identify, in the old parlance of IUH theory, the concentration time of a particular catchment under its specific climate history.

Niemi's identity, on the other hand, shows that if the BTTD are affected by celerity then so should the hydrologic response be.

5 The Swiss Army knife for understanding

The Swiss Army knife for understanding all of the above relationships is given by the decomposition of both the backward and forward probabilities in terms of the age-ranked discharges (van der Velde et al., 2012; Benettin et al., 2013; Harman, 2019), which are actually the functions tabulated in Figure 1. The s-table in the figure is a discrete representation of the age-ranked storage, $s(t, t_i)$, for which:

$$S(t) = \sum_{\forall t_i} s(t, t_i) \tag{6}$$

where $S(t)$ is the total water present in the control volume. The age ranked discharges, $q(t, t_i)$, are represented in the q-table and for them a relation similar to equation (6) is valid. They represent the decomposition of a given discharge according to the ages that compose it (or, which is equivalent, the precipitation time). All the details of these decomposition can be found, for instance, in Rigon, Bancheri, and Green (2016). Here we give a brief compendium based on Figure 1 where the entries of the q-table are the age-ranked discharge recorded at discrete times. If we focus just on new water and old water, these can be obtained by separating the columns of the q-table in the figure into two groups, before and after a certain date t_i (included), and the columns entries summed together.

The use of age-ranked functions not only makes Niemi's identity trivial, corresponding to the intersection of a given column (from which the IUH is obtained) and a given row (from which the BTTD is obtained) in the q-table, but also suggests easy numerical methods for the computation of any of the quantities presented in the previous descriptions.

6 Conclusions

The result of the above findings, well described in Benettin et al. (2022), is that in recent years a great number of papers have embraced the new insights for investigating how water moves in hillslopes, either using the approach shown in Kirchner (2019) or the SAS approach. Using process-based approaches, database approaches and their variations (Meira Neto et al., 2022), it has been possible to determine that transport mechanisms vary greatly between wet and dry periods, due to the interplay of surface runoff, soil flow and groundwater contribution (Soulsby et al., 2015; Tetzlaff et al., 2014; Wilusz et al., 2017; von Freyberg et al., 2017; Knapp et al., 2019). Various papers, as reported in Benettin et al. (2022), have described the mechanism of activation of flows of old water and the impact of new precipitation.

Besides, the indications derived from the new T3 approaches are also affecting the way catchments are modelled. Because it has been shown that to any model structure there corresponds a travel time signature (Rigon & Bancheri, 2021), the model-used-as-hypothesis approach (Clark et al., 2011; Beven, 2018) has acquired new tools to be exploited.

As emphasized in the last sections of Benettin et al. (2022), using T3 allows for more than just predicting discharges of water and solutes. It opens new directions for the investigation of the whole hydrological cycle (McDonnell, 2014), especially in assessing how vegetation uses water of different ages.

Eventually, these and others new challenges are carefully reviewed in Benettin et al. (2022) opening up, as Li et al. (2021) states, to the development of integrated Earth system science theories at the intersection of hydrology, biology and geochemistry, following the call for understanding of climate-soil-vegetation dynamics that started with Rodriguez-Iturbe (2000).

Acknowledgments

All the Authors contributed equally to this commentary. It was partially financed by the WATERSTEM PRIN project. A few videos were prepared to illustrate the concepts of the commentary, which can be found here: https://vimeo.com/showcase/10101034

References

Benettin, P., Rinaldo, A., & Botter, G. (2013, December). Kinematics of age mixing in advection-dispersion models. *Water Resour. Res.*, *49*(12), 8539–8551.

Benettin, P., Rodriguez, N. B., Sprenger, M., Kim, M., Klaus, J., Harman, C. J., ... McDonnell, J. J. (2022, November). Transit time estimation in catchments: Recent developments and future directions. *Water Resour. Res.*, *58*(11).

Benettin, P., Soulsby, C., Birkel, C., Tetzlaff, D., Botter, G., & Rinaldo, A. (2017, March). Using SAS functions and high-resolution isotope data to unravel travel time distributions in headwater catchments. *Water Resour. Res.*, *53*(3), 1864–1878.

Beven, K. J. (2018, May). On hypothesis testing in hydrology: Why falsification of models is still a really good idea. *WIREs Water*, *5*(3), e1278.

Botter, G., Bertuzzo, E., & Rinaldo, A. (2010, March). Transport in the hydrologic response: Travel time distributions, soil moisture dynamics, and the old water paradox. *Water Resour. Res.*, *46*(3).

Botter, G., Bertuzzo, E., & Rinaldo, A. (2011, January). Catchment residence and travel time distributions: The master equation. *Geophys. Res. Lett.*, *38*(11).

Clark, M. P., Kavetski, D., & Fenicia, F. (2011, September). Pursuing the method of multiple working hypotheses for hydrological modeling. *Water Resour. Res.*, *47*(9).

Dagan, G. (1986, September). Statistical theory of groundwater flow and transport' pore to laboratory, laboratory to formation, and formation to regional scal. *Water Resour. Res.*, *22*(9), 120–134.

Dooge, J. C. I. (1986, August). Looking for hydrologic laws. *Water Resour. Res.*, *22*(9S), 46S–58S.

Durighetto, N., & Botter, G. (2022, July). On the relation between active network length and catchment discharge. *Geophys. Res. Lett.*, *49*(14), e2022GL099500.

Godsey, S. E., & Kirchner, J. W. (2014, November). Dynamic, discontinuous stream networks: hydrologically driven variations in active drainage density, flowing channels and stream order. *Hydrol. Process.*, *28*(23), 5791–5803.

Harman, C. J. (2015, January). Time-variable transit time distributions and transport: Theory and application to storage-dependent transport of chloride in a watershed. *Water Resour. Res.*, *51*(1), 1–30.

Harman, C. J. (2019, August). Age-ranked storage-discharge relations: A unified description of spatially lumped flow and water age in hydrologic systems. *Water Resour. Res.*, *55*(8), 7143–7165.

Kirchner, J. W. (2019, January). Quantifying new water fractions and transit time distributions using ensemble hydrograph separation: theory and benchmark tests. *HESS*, *23*, 303–349.

Klaus, J., & McDonnell, J. J. (2013, November). Hydrograph separation using stable isotopes: Review and evaluation. *J. Hydrol.*, *505*(C), 47–64.

Knapp, J. L. A., Neal, C., Schlumpf, A., Neal, M., & Kirchner, J. W. (2019, June). New water fractions and transit time distributions at plynlimon, wales, estimated from stable water isotopes in precipitation and streamflow. *Hydrol. Earth Syst. Sci. Discuss.*, 1–40.

Li, L., Sullivan, P. L., Benettin, P., Cirpka, O. A., Bishop, K., Brantley, S. L., ... Kirchner, J. W. (2021, January). Toward catchment hydro-biogeochemical theories. *WIREs Water*, *8*(1).

Maloszewski, P., & Zuber, A. (1996, October). *Lumped parameter models for the interpretation of environmental tracer data* (Tech. Rep.).

McDonnell, J. J. (2014, April). The two water worlds hypothesis: ecohydrological separation of water between streams and trees? *Wiley Interdisciplinary Reviews: Water*.

McDonnell, J. J., & Beven, K. (2014, June). Debates-The future of hydrological sciences: A (common) path forward? a call to action aimed at understanding velocities, celerities and residence time distributions of the headwater hydrograph. *Water Resour. Res.*, *50*(6), 5342–5350.

McGuire, K. J., & McDonnell, J. J. (2006, November). A review and evaluation of catchment transit time modeling. *J. Hydrol.*, *330*(3), 543–563.

Meira Neto, A. A., Kim, M., & Troch, P. A. (2022, February). Physical interpretation of time-varying StorAge selection functions in a bench-scale hillslope experiment via geophysical imaging of ages of water. *Water Resour. Res.*.

Nauman, E. B. (1969, June). Residence time distribution theory for unsteady stirred tank reactors. *Chem. Eng. Sci.*, *24*, 1471–1480.

Niemi, A. J. (1977, October). Residence time distributions of variable flow processes. *Int. J. Appl. Radiat. Isot.*, *28*(10), 855–860.

Rigon, R., & Bancheri, M. (2021, January). On the relations between the hydrological dynamical systems of water budget, travel time, response time and tracer concentrations. *Hydrol. Process.*, *35*(1).

Rigon, R., Bancheri, M., Formetta, G., & de Lavenne, A. (2016, January). The geomorphological unit hydrograph from a historical-critical perspective. *Earth Surf. Processes Landforms*, *41*(1), 27–37.

Rigon, R., Bancheri, M., & Green, T. R. (2016, May). Age-ranked hydrological budgets and a travel time description of catchment hydrology. *Hydrol. Earth Syst. Sci. Discuss.*, 1–22.

Rinaldo, A., Benettin, P., Harman, C. J., Hrachowitz, M., McGuire, K. J., van der Velde, Y., . . . Botter, G. (2015, June). Storage selection functions: A coherent framework for quantifying how catchments store and release water and solutes. *Water Resour. Res.*, *51*(6), 4840–4847.

Rodriguez-Iturbe, I. (2000). Ecohydrology: A hydrologic perspective of climate-soil-vegetation dynamics. *Water Resources Research*, *36*(1).

Rodriguez-Iturbe, I., & Valdes, J. B. (1979). The geomorphologic structure of the hydrologic response. *Water Resources Reesearch*, *15*(6), 1409–1420.

Soulsby, C., Birkel, C., Geris, J., Dick, J., Tunaley, C., & Tetzlaff, D. (2015, September). Stream water age distributions controlled by storage dynamics and nonlinear hydrologic connectivity: Modeling with high-resolution isotope data. *Water Resour. Res.*, *51*(9), 7759–7776.

Tetzlaff, D., Buttle, J., Carey, S. K., McGuire, K., Laudon, H., & Soulsby, C. (2014, December). Tracer-based assessment of flow paths, storage and runoff generation in northern catchments: a review. *Hydrol. Process.*, *29*(16), 3475–3490.

van der Velde, Y., Torfs, P. J. J. F., Van der Zee, S. E. A. T. M., & Uijlenhoet, R. (2012, June). Quantifying catchment-scale mixing and its effect on time-varying travel time distributions. *Water Resour. Res.*, *48*(6), W06536–13.

von Freyberg, J., Studer, B., & Kirchner, J. W. (2017, March). A lab in the field: high-frequency analysis of water quality and stable isotopes in stream water and precipitation. *Hydrol. Earth Syst. Sci.*, *21*(3), 1721–1739.

Wilusz, D. C., Harman, C. J., & Ball, W. P. (2017, December). Sensitivity of catchment transit times to rainfall variability under present and future climates. *Water Resour. Res.*, *53*(12), 10231–10256.