ORIGINAL ARTICLE

Journal Section

Equivalences and differences between the hydrological dynamical systems of water budget, travel time, response time, and tracer concentrations and the legacy of models' topology

Riccardo Rigon*[1] | Marialaura Bancheri[2]

[1]Department of Civil, Environmental e Mechanical Engineering, University of Trento, Via Mesiano, 77, 38123 Trento, Italy

[2]Institute for Agricultural and Forest Systems in the Mediterranean, National Research Council, Via Patacca, 85, 80056 Ercolano NA, Italy

Correspondence
*Riccardo Rigon, Department of Civil, Environmental e Mechanical Engineering, University of Trento, Via Mesiano, 77, 38123 Trento, Italy
Email: riccardo.rigon@unitn.it

Funding information
PRIN 2017 WATZON

We present, by using previous results on extended Petri Nets, the relations of various hydrological dynamical systems (`HDSys`) derived from the water budget (`DynWB`). Once `DynWB` has been implemented, there exist a consistent way to get the equations for backward travel time distributions (`DynTT`), for the forward response time distribution (`DynRTD`) and for the concentration for a solute or a tracer (`DynC`). We show that the `DynWB` has a correspondence one to many with the `DynTT`. In fact to any one of the `DynWB` equation correspond as many equation as the input precipitation events times. The `DynTT` is related to `DynRTD` by the Niemi's relationship and, in presence of multiple, n outputs, by the specification of $n-1$ partition functions, which determine which fraction of water volume, injected in the control volume at a specific time t_{in}, goes asymptotically into a specific output. The `DynC`, given `DynTT`, depends further on the solute/tracer concentration in inputs. The paper clarifies the complicate set of relations above by using an example from literature. Upon the introduction of the appropriate information, it is also shown how these (`HDSys`) can be solved simultaneously without duplicating calculations. It is also shown that these systems can be solved exactly, under the hypothesis of uniform mixing of water ages inside each reservoir within the system.

KEYWORDS
Extended Petri Nets; Hydrological dynamical systems; Travel times; Response times; Tracer concentrations

1 | INTRODUCTION

The extended Petri Nets (EPN), presented in a previous paper by Bancheri et al. (2019), are a new way to describe the hydrological water and energy budgets with graphs. EPN, more than a pictorial representation, are actually a notation for the systems' equations themselves. Any hydrological dynamical systems (HDSys) was seen to be composed by a topology and a semantics, the first describing the connections between the compartments of the budget, and the second associating symbols to the topology, a meaning to symbols and an expression to fluxes, as overviewed in Appendix A.

In this paper we use EPN to discuss various aspects of the water budget (named from now on `DynWB` as Dynamical Water Budget) and discuss its relationship with other dynamical systems, namely:

- travel times (Maloszewski and Zuber, 1982; McGuire and McDonnell, 2006; Sprenger et al., 2019), described by the age-ranked functions, as in Rigon et al. (2016b). This dynamical system will be named `DynTTD` as Dynamical system of backward Travel Times Distribution, according to Botter et al. (2010, 2011);
- response times that generalizes the geomorphological unit hydrograph theory Rodríguez-Iturbe and Valdes (1979); Gupta and Waymire (1983); Rodríguez-Iturbe and Rinaldo (2001); Rigon et al. (2016a,b). This dynamical system will be named `DynRTD` as Dynamical system of Response Time Distribution;
- solute/tracers concentrations, named `DynC` as Dynamical system of Concentrations McGuire and McDonnell (2006); Duffy (2010).

To show these equivalences, we borrow some concepts from the language of the category theory (Fong and Spivak, 2018). We do not introduce category theory here explicitly, in order to maintain our description as simple as possible, but interested readers should refer to (Rihel, 2016; Fong and Spivak, 2018; Bradley, 2018). However, we will define and mention below the concept of functor (e.g., Bradley (2018)), a "function" that connects every element of a dynamical system with the correspondent of the other dynamical systems, i.e. the state variables with the state variable, but also the fluxes with the fluxes, and any quantity that appears in the mathematical description of one HDSys.

Our methodology for discussing the relations among the four dynamical systems (DynWB, Dyn TTD, DynRTD and DynC) is based on:

1. showing that HDSys are representable as EPN;
2. exploiting these facts by describing each system through the graphical representation;
3. adding the dictionary and the various expression tables, relative to each HDSys in such a way that there is a one to one correspondence between the differential or integral operators of each system.

Points one and two above are essentially already accomplished in Figure 1) and therefore what remains to do is to write the dictionaries and the tables of expression for all the HDSys. With the latter operations, we practically construct the functors that connects the categories, i.e. we give the rules to associate reservoir (called *object* in category theory, *place* in EPN) to reservoir between two HDSys and flux (called *arrow* in category theory, *transition* in EPN) to flux. Practically the equivalences come automatically, as a demonstration of the power of EPN representation, by associating the same numbered rows of the dictionaries and table of expression.

The association/equivalence seems therefore a straightforward achievement but less trivially we will produce also the mathematical expression of the solutions of the dynamical systems and highlight that the mathematical morphism

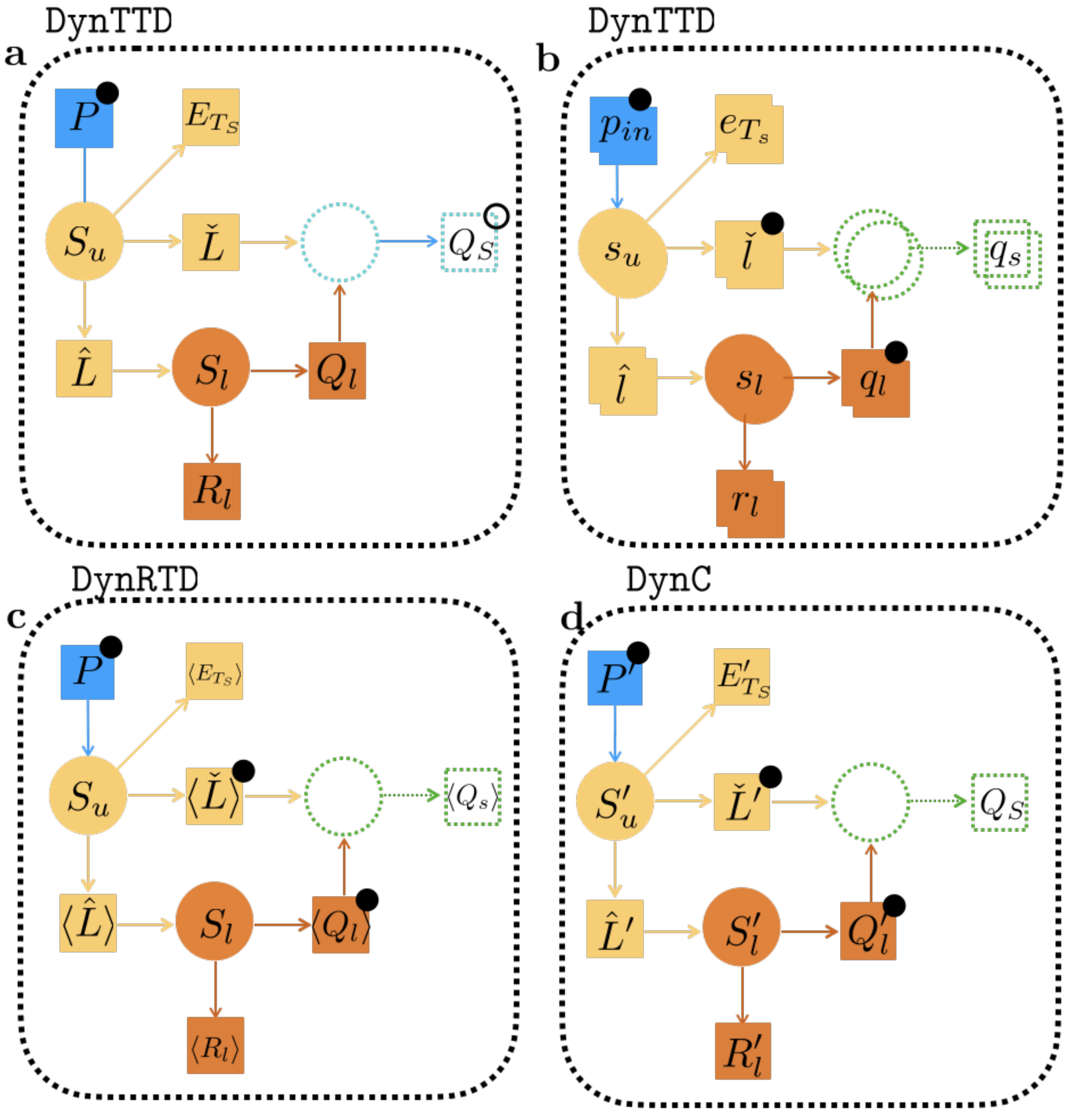

FIGURE 1 Based on the same topology, we can have different view of our perceptual model. On top left (DynWB) we have the EPN representation of the water budget of a subbasin of the Maimai catchment (Gabrielli et al., 2018) or the model used in (Kirchner, 2016, 2019); on top right (Dyn TTD) we have the representation of the travel time distributions; on bottom left (DynRTD) we have the representation of the life expectancy distributions; on bottom right (DynC) we have the representation of the concentrations of a tracer.

between the dynamical systems is not a isomorphism because the information content of any of the system is slightly different and some assumptions, usually buried below the mathematical formalism, must be done to move from one to the the other.

To exemplify the concepts just enumerated, we start from discussing the `DynWB`, which is the basis of all of our arguments.

2 | THE WATER BUDGET `DynWB`

We firstly illustrate the water budget, assuming that it is representative of some really existent hydrological system, and, for instance, the Maimai catchment (Gabrielli et al., 2018) could be such a case. One aspect of EPN is that they have a topological part, called topology of the model, which resolves the system behavior in a group of interconnected reservoirs (absolutely the same way the tradition teaches, (Beven, 2011)) that receive and exchange fluxes and a more specific part that represents the mathematical expressions used for estimating the fluxes (the semantic of the model). Concentrating our attention to Figure 1, the reservoirs are represented by two circles, and corresponds to the number of ODEs used. Squares represents the fluxes between the reservoirs or inputs or outputs. The dotted line circle is a stationary reservoir where waters from S_u and S_l just mix to produce the discharge Q_S as a sum of contributions.

As already mentioned, in the EPN nomenclature Bancheri et al. (2019), the reservoirs (circles) are named **places** and the fluxes **transitions**. The **dictionary** of dynamical system in Table 1 gives a meaning to the variables used. Differently from Bancheri et al. (2019), we number here the row of the dictionary for use in the following sections.

#	Symbol	Name	Type	Unit
1	E_{T_S}	Evapotranspiration	F	[L T^{-1}]
2	$\hat{L}$	Percolation from upper storage to lower storage	F	[L T^{-1}]
3	$\check{L}$	Discharge from the upper reservoir	F	[L T^{-1}]
4	P	Precipitation	F	[L T^{-1}]
5	Q_l	Discharge from the lower reservoir	F	[L T^{-1}]
6	Q_S	Surface water discharges	F	[L T^{-1}]
7	R_l	Percolation flux to deeper groundwater	F	[L T^{-1}]
8	S_l	Lower storage reservoir	SV	[L]
9	S_u	Water upper storage	SV	[L]

TABLE 1 Dictionary of the HDSys presented in Figure 1 a). F stand for "flux"; SV stands for "State Variable"; [L] for "length unit"; [T] for "time" unit. The names of the variables were chosen after (Kirchner, 2016).

Before translating the graph to equations, we have to specify a table of expression for the places, to associate to any place symbol an operator, as shown in Table 2 below.

After the use of Expression in Table 2, the diagram in Figure 1 allows the writing of the systems' equations as:

$$\frac{dS_u(t)}{dt} = P(t) - E_{T_s}(t) - \check{L}(t) - \hat{L}(t) \tag{1}$$

#	Symbol	Name	Expression
8	S_l	Water in lower storage	dS_l/dt
9	S_u	Water in the upper storage	dS_u/dt

TABLE 2 Expression for the Water Budget places. The numbers refer to the position of the state variable in the dictionary of Table 1

$$\frac{dS_l(t)}{dt} = \hat{L}(t) - Q_l(t) - R_l(t) \tag{2}$$

$$Q_S(t) = Q_l(t) + \check{L}(t) \tag{3}$$

As written in Table 2 to the state variables in place S_l and S_u correspond, in the left side of the equations, the time variation of the quantity. At the right side of the equation, transitions with an input arrow going into the place are positive, and transitions, with an output arrow going out the place are negative. So, for the upper reservoir, precipitation, P, is an input while there are three outputs, E_{T_s}, $\check{L}$ and $\hat{L}$. The dashed, unnamed place is then used to show that low and upper reservoir discharges mix and are collected in surface water. In turn, the surface water reservoir does not vary its water content and its outputs is exactly the sum of the incoming discharges (for these reasons the reservoir is dashed, or *invisible*.

These water budget equations are not fully specified and cannot be solved, since the fluxes' expressions are not yet given. In this case, Kirchner (2016, 2019) help us to build our example and giving an expression for each input and output flux. The expressions are given below in Table 3 which, for its function, is called *Expression Table* of the model.

Symbol	Name	Expression	
1	E_{T_S}	Evapotranspiration	$f(R_n, u, \delta e, T_a, z_d, z_0)$
2	$\hat{L}$	Percolation from upper storage to lower storage	$(1-\eta)k_u S_u^{b_u}$
3	$\check{L}$	Discharge from the upper reservoir	$\eta k_u S_u^{b_u}$
4	P	Precipitation	•
5	Q_l	Discharge from the lower reservoir	$\beta k_l S^{b_l}$
6	Q_S	Total discharge	$\check{L} + Q_l$
7	R_l	Percolation flux to deep groundwater	$(1-\beta)k_l S^{b_l}$

TABLE 3 Expressions of fluxes from and into reservoirs. With respect to Kirchner (2016), evapotranspiration and percolation to deep groundwater were added to be more similar to the Gabrielli et al. (2018) perceptual model. Evapotranspiration expression was not actually specified but thought as function of net radiation, R_n, wind velocity, u, evaporative demand, δe, air temperature, T_a, zero displacement height, z_d and surface roughness, z_0. The • symbol indicates that precipitation are measured, i.e. a given quantity.

An ancillary dictionary should be then produced to explain all the new symbols introduced. Table 4 contains it

Symbol	Name	Type	Unit
b_l	Parameter in Q_l expression	P	[-]
b_u	Parameter in $\hat{L}$ and $\check{L}$ expression	P	[-]
k_l	Lower reservoir coefficient	P	[T^{-1} L$^{1-b_l}$]
k_u	Upper reservoir coefficient	P	[T^{-1} L$^{1-b_u}$]
R_n	Net Radiation	V	[E T^{-1} L^{-2}]
T_a	Air temperature	V	[K]
u	wind velocity	V	[L T−1]
z_0	Surface roughness	P	[L]
z_d	Zero displacement height	P	[L]
β	Partition coefficient for lower reservoir fluxes	P	[-]
δe	Evaporative demand	V	[F L^{-2}]
η	Partition coefficient for the upper reservoir fluxes	P	[-]

TABLE 4 Additional dictionary introduced after the explication of fluxes in 3. To be added to Table 1

with mostly parameters to be set by literature knowledge or calibration values.

The dynamical system such defined can be solved numerically once precipitation and evaporation data are available. Evaporation, in turn, could be obtained by making explicit the model used, i.e. the form of the function f in Table 3. This is not necessary at present and we avoid it for simplicity. However, from now on, we will assume that all the state variable, $S_u(t)$ and $S_l(t)$ are known for all the instant of time for which we have precipitations inputs. A larger set of model's examples, to which, the same considerations apply are presented in Bancheri et al. (2019).

3 | THE TRAVEL TIME `DynTTD`

With just a simple change of semantics, the same topology of Figure 1 a) can represent travel time distributions Rigon et al. (2016b), as shown in Figure 1 b).

The main visible changes in Figure 1 b) are i) the addition of shadows to the graph, to indicate that we are now dealing with a system of equations, each one dependent on a t_{in}, i.e. the injection time to the control volume and ii) the use of lower case quantities. The dictionary of the `DynTTD` system is presented below in Table 5.

Each of the quantities appearing in Table 5 are **age-ranked** functions, i.e. they trace the quantity of water injected in the system with precipitation at time t_{in}. Once integrated over the injection time, they give the corresponding ‘bulk" quantities present in Table 1. For instance, it is:

$$S_l(t) = \int_{-\infty}^{t} s_l(t, t_{in}) dt_{in} \tag{4}$$

where S_l is the eightest entry in Table 1 and $sl(t, t_{in}$ is the eightest entry in Table 5. The complete treatment of the theory, mainly due to Botter et al. (2010) and van der Velde et al. (2012), is presented in Rigon et al. (2016b) with the

#	Symbol	Name	Type	Unit
1	$e_{TS}(t, t_{in})$	Evapotranspiration generated by p_{in}	F	[L T^{-2}]
2	$\hat{I}(t, t_{in})$	Percolation from upper storage generated by p_{in}	F	[L T^{-2}]
3	$\check{I}(t, t_{in})$	Discharge from the upper reservoir generated by p_{in}	F	[L T^{-2}]
4	$p_{in}(t_{in})$	Precipitation at time t_{in}	F	[L T^{-2}]
5	$q_l(t, t_{in})$	Discharge from the lower reservoir generated by p_{in}	F	[L T^{-2}]
6	$q_s(t, t_{in})$	Surface water discharge generated by p_{in}	F	[L T^{-2}]
7	$r_l(t, t_{in})$	Percolation flux to deeper groundwater generated by p_{in}	F	[L T^{-2}]
8	$s_l(t, t_{in})$	Water in lower storage generated by by p_{in}	SV	[L T^{-1}]
9	$s_u(t, t_{in})$	Water in upper storage by p_{in}	SV	[L T^{-1}]

TABLE 5 Dictionary of the DynTTD. The enumerated quantities are all age-ranked functions, since the dependence from the injection time t_{in} has been added

same notation we use in this paper. Equations are obtained by associating the differential operator to state variables, as shown in Table 6, analogously to what already done in the case of `DynWB`:

Symbol	Name	Expression	
8	s_l	Water in lower storage	$ds_l(t, t_{in})/dt$
9	s_u	Water in the upper storage	$ds_u(t, t_{in})/dt$

TABLE 6 Expression for age ranked state variable. The numbers refer to the position of the state variable in the dictionary of Table 5

Therefore the age-ranked equations for the Kirchner (2016) system are:

$$\frac{ds_u(t, t_{in})}{dt} = p_{in}(t_{in}) - e_{T_S}(t, t_{in}) - \check{I}(t, t_{in}) - \hat{I}(t, t_{in}) \tag{5}$$

and

$$\frac{ds_l(t, t_{in})}{dt} = \hat{I}(t, t_{in}) - r_l(t, t_{in}) - q_l(t, t_{in}) \tag{6}$$

with also:

$$q_s(t, t_{in}) = \check{I}(t, t_{in}) + q_l(t, t_{in}) \tag{7}$$

In the theory of age-ranked functions, the expressions to insert into fluxes variables are not given directly but are mediated by the introduction of the so called backward residence time probabilities, defined as:

$$p_i(t - t_{in}|t) := \frac{s_i(t, t_{in})}{S(t)} \tag{8}$$

where $i \in \{u, l\}$ means that i can be either u or l, and the backward travel time probabilities:

$$p_k(t - t_{in}|t) := \frac{g(t, t_{in})}{G(t)} \tag{9}$$

where $(g, G) \in \{(e_{T_S}, E_{T_S}), (\check{I}, \check{L}), (\hat{I}, \hat{L}), (r_l, R_l), (q_l, Q_l)\}$, meaning that any of the couples between the braces can be substututed to (g, G). Furthermore, according to Botter et al. (2010, 2011), the following equation is valid:

$$p_k(t - t_{in}|t) := \omega_{ki}(t, t_{in}) p_i(t - t_i in|t) \tag{10}$$

where, if $k \in \{e_{T_S}, \hat{I}, \check{I}\}$, then $i = u$ or, if $k \in \{q_l, r_l\}$, then $i = l$, and ωs are called StoraAge Selection functions (SAS).

Substitution of (8) into (5) gives:

$$\begin{aligned} \frac{dS_u(t) p_u(t - t_{in}|t)}{dt} = \quad & p_{in}(t_{in})\delta(t - t_{in}) - E_{T_S}(t)\omega_{T_S}(t, t_{in}) p_u(t - t_{in}|t) + \\ & -\check{L}(t)\omega_{\check{L}}(t, t_{in}) p_u(t - t_{in}|t) - \hat{L}(t)\omega_{\hat{L}}(t, t_{in}) p_u(t - t_{in}|t) \end{aligned} \tag{11}$$

and substitution of (9) into (6) gives:

$$\frac{dS_l(t) p_l(t - t_{in}|t)}{dt} = \hat{L}(t)\omega_{\hat{L}}(t, t_{in}) p_u(t - t_{in}|t) - Q_l(t)\omega_{Q_l}(t, t_{in}) p_l(t - t_{in}|t) - R_l(t)\omega_{R_l}(t, t_{in}) p_l(t - t_{in}|t) \tag{12}$$

After Equations (11) and (12) we can reshape the association rule for the differential operator acting on state variables. In place of Table 6, we better use:

Symbol	Name	Expression	
8	s_l	Water in lower storage	$dS_l(t) p_l(t - t_{in}|t)/dt$
9	s_u	Water in the upper storage	$dS_u(t) p_u(t - t_{in}|t)/dt$

TABLE 7 Operators to apply to age ranked state variables, for obtaining Equations (11) and (12)

We are also ready to properly write the expression table for transitions in the age-ranked equations, as reported in Table 8.

With Tables 7 and 8 we have completed the construction of the functor relating the `DynWB` and `DynTTD` dynamical systems. In fact, we have simply to associate the rows of the related tables to obtain the correspondence:

- among symbols, associating Table 1 as domain to Table 5 as codomain;
- among operators, associating Table 2 as domain to Table 6 as codomain;

Symbol	Name	Expression	
1	e_{T_S}	Age-ranked evapotranspiration	$E_{T_S}(t)\omega_{e_{T_S}}(t,t_{in})p_u(t-t_{in}\|t)$
2	$\hat{l}$	Age-ranked percolation	
		for upper storage to lower storage	$\hat{L}(t)\omega_{\hat{L}}(t,t_{in})p_u(t-t_{in}\|t)$
3	$\check{l}$	Age-ranked discharge from the upper reservoir	$\check{L}(t)\omega_{\check{L}}(t,t_{in})p_u(t-t_{in}\|t)$
4	p_{in}	Precipitation input a time t_{in}	•
5	q_l	Age-ranked discharge from lower reservoir	$\check{Q}_l(t)\omega_{Q_l}(t,t_{in})p_l(t-t_{in}\|t)$
6	q_s	Age-ranked total discharge	$q_l(t,t_{in})+q_s(t,t_{in})$
7	r_l	Age-ranked percolation flux to groundwater	$\check{R}_l(t)\omega_{R_l}(t,t_{in})p_l(t-t_{in}\|t)$

TABLE 8 Expression of the operators to apply to age ranked state variables, for obtaining Equations (11) and (12)

- among expressions, associating Table 3 as domain to Table 8 as codomain.

Notwithstanding this morphism between the two HDSys, they do not contain the same information. To obtain the dynamics of `DynTTD` we have, in fact, to specify the form of the SAS functions which require further knowledge or assumptions. Besides, the morphism is a relation one-to-many, since to each equation in `DynWB` correspond a set of equations in `DynTTD`, each one labeled ("ranked") by a precipitation time t_{in}. At the same time, for solving `DynTTD`, the knowledge of the solutions of `DynWB` is mandatory, since the bulk quantities appear explicitly in the age-ranked equations.

Equations (11) and (12) are linear in the probabilities $p_l(t-t_{in}|t)$ and $p_u(t-t_{in}|t)$ and are analytically solvable (Botter et al., 2010, 2011).

During the recent years various recipes were developed to constrain the form of the SAS (e.g., Benettin et al. (2017)), however in many papers, the simplest assumption is made that the fluxes are sampled uniformly from the storages and, i.e., $\forall i\ \omega_i(t,t_{in})=1$. In this case the solutions for the probabilities p_u is (Botter et al., 2010):

$$p_u(t-t_{in}|t)=\frac{P(t_{in})}{S_u(t_{in})}e^{-\int_{t_{in}}^{t}\frac{P(t')}{S_u(t')}dt'} \tag{13}$$

while the solution for the probability p_l, after applying the rules for integration of a linear ODE, as provided in the complimentary material, results:

$$p_l(t-t_{in}|t)=\frac{P(t_{in})}{S_u(t_{in})}\int_{t_{in}}^{t}\frac{\hat{L}(t'')}{S_l(t'')}e^{-\int_{t_{in}}^{t''}\frac{P(t')}{S_u(t')}dt'}e^{-\int_{t''}^{t}\frac{\hat{L}(t')}{S_l(t')}dt'}dt'' \tag{14}$$

Upon defining:

$$p_l(t-t''|t):=\frac{\hat{L}(t'')}{S_l(t'')}e^{-\int_{t''}^{t}\frac{\hat{L}(t')}{S_l(t')}dt'} \tag{15}$$

which can be seen as the backward probability distribution of travel time inside the single place S_l, equation 14 can be written as:

$$p_l(t - t_{in}|t) = \int_{t_{in}}^{t} p_l(t - t''|t) p_u(t'' - t_{in}|t'') dt'' := \langle p_l * p_u \rangle \tag{16}$$

which contains a sort of convolution between the travel times inside the path $S_u \rightarrow S_l$. This is actually not a convolution of probabilities in strict sense, since, while p_l is a probability distribution function (pdf) in t'', p_u is a probability distribution function in t_{in} and not in t'' Rigon et al. (2016b). This is the reason why we indicated this operation in (16) with the $\langle$ and $\rangle$ parentheses besides the traditional $*$ sign.

4 | THE RESPONSE ORIENTED `DynRTD`

A traditional way to mathematically describe the water fluxes is given by the theory of instantaneous unit hydrograph and its generalizations Beven (2011); Rigon et al. (2016a). In the supplementary material with practical example, we show how this HDSys deals with the *life expectancy*, i.e., the time at which one molecule of water is expected to exit the control volume, which is a variable shared with populations dynamics (e.g., Calabrese and Porporato (2015)). We do not require a new dictionary for this dynamical system, as it is evident from the Figure 1 c) that uses for places the same symbols of Figure 1 a). Not even a new operators table is required, since the budget equations remain the same as in equations Equations 1 and 2. Fluxes are instead represented by the same symbols than in `DynWD` but with $\langle$ and $\rangle$ parentheses, because, in these theories fluxes are assigned through a convolution:

$$\langle \hat{Q}_{kji} \rangle = \int_{-\infty}^{t} \underbrace{\Theta_{ki}(t_{in}) p_k(t - t_{in}|t_{in})}_{\mathcal{F}(t,t_{in})} J_{jk}(t_{in}) dt_{in} := [p_{ki} * (\Theta_{ki} J_{jk})](t) \tag{17}$$

where

- $J_{jk}(t_{in})$ is the j-est input to the k storage;
- $p_k(t - t_{in}|t_{in})$ is the so called response time probability or life expectation probability (conditional on t_{in}) of the k-est storage;
- $\Theta_{ki}(t_{in})$ is a coefficient that partitions the outgoing fluxes and was found to be dependent of the injection time t_{in} Botter et al. (2010);
- $\langle \hat{Q}_{kji} \rangle$ is the i-est outgoing flux from storage (place) k generated by the $j - est$ input;
- $\mathcal{F}(t, t_{in})$ is the known response function, whose meaning will be explained below.

In the hydrological literature (e.g., Rigon et al. (2016a)), the treatment of these system is obtained by assigning the probabilities $p_k(t - t_{in}|t_{in})$ instead of solving the partial differential equations of the water budget. Actually, if we start by solving `DynWB` we can, for any time t, determine $\mathcal{F}$ but its separation in Θ_{ki} and p_k can be determined only at $t = \infty$ as described in Rigon et al. (2016b). The square parentheses and the * symbol are used as a short form for the convolution represented by the integral. Therefore the expression table for `DynRTD` is now changed as shown in Table 9, where it is to be noticed that the convolutions contain also the partitioning functions Θ_{ki}.

#	Symbol	Name	Expression
1	$\langle E_{T_S} \rangle$	Evapotranspiration	$[p_{E_{T_S}} * (\Theta_{E_{T_S}} P)]$
2	$\langle \hat{L} \rangle$	Percolation from upper storage to lower storage	$[p_{\hat{L}} * (\Theta_{\hat{L}} P)]$
3	$\langle \check{L} \rangle$	Discharge from the upper reservoir	$[p_{\check{L}} * (\Theta_{\check{L}} P)]$
4	P	Precipitation	•
5	$\langle Q_l \rangle$	Discharge from the lower reservoir	$[p_{Q_l} * (\Theta_{Q_l} \hat{L})] = [p_{Q_l} * (\Theta_{Q_l} * p_{\hat{L}} * (\Theta_{\hat{L}} P))]$
6	$\langle Q_S \rangle$	Total discharge	$\check{L} + Q_l$
7	$\langle R_l \rangle$	Percolation flux to deep groundwater	$[p_{R_l} * (\Theta_{R_l} \hat{L})] = [p_{R_l} * (\Theta_{R_l} * p_{\hat{L}} * (\Theta_{\hat{L}} P))]$

TABLE 9 The dynamical system `DynRTD` is given trough the assignment of the response time distribution of the fluxes.

In `DynRTD` the bulks mass budget for the u reservoir can be written as:

$$\frac{dS_u}{dt} = P(t) - [p_{E_{T_S}} * (\Theta_{E_{T_S}} P)](t) - [p_{\check{L}} * (\Theta_{\check{L}} P)](t) - [p_{\hat{L}} * (\Theta_{\hat{L}} P)](t) \tag{18}$$

where, for instance, is:

$$[p_{\hat{L}} * (\Theta_{\hat{L}} P)](t) := \int_{-\infty}^{t} \underbrace{p_{\hat{L}}(t - t_{in}|t_{in})(\Theta_{\hat{L}}(t_{in})}_{\mathcal{F}_{\hat{L}}(t,t_{in})} P(t_{in}))dt_{in} \tag{19}$$

and analogous equations hold for the other outgoing fluxes $\check{L}$ and E_{T_S}. For the l reservoir is therefore:

$$\frac{dS_l}{dt} = [p_{\hat{L}} * (\Theta_{\hat{L}} P)] - [p_{Q_l} * (\Theta_{Q_l} * p_{\hat{L}} * (\Theta_{\hat{L}} P))] - [p_{R_l} * (\Theta_{R_l} * p_{\hat{L}} * (\Theta_{\hat{L}} P))] \tag{20}$$

where, is:

$$[p_{R_l} * (\Theta_{R_l} p_{\hat{L}} * (\Theta_{\hat{L}} P))] := \int_{-\infty}^{t} p_{R_l}(t-\tau)\Theta_{R_l}(\tau) \underbrace{\left[\int_{-\infty}^{\tau} p_{\hat{L}}(\tau - \epsilon|\epsilon)\Theta_{\hat{L}}(\epsilon)P(\epsilon)\, d\epsilon\right]}_{\hat{L}(\tau)} d\tau \tag{21}$$

If the response probabilities are assigned, the water budget is known, and therefore there is a clear functor between `DynRTD` and `DynWB`. Evidently, the assignment of `DynRTD` expressions of Table 9 is usually not compatible with the contemporary assignment of an expression for fluxes. In fact, equating for instance row 2 of Table 3 and Table 9, produces:

$$(1-\eta)K_u S_u^{b_u} = [p_{\hat{L}} * (\Theta_{\hat{L}} P)] \tag{22}$$

a functional equation that cannot be guaranteed to be satisfied for an arbitrary form of the right member of Equation 22 and for any time. Vice versa, assignment of fluxes of the water budget implicitly determines the expression of the response probabilities. Because, as said above, at any time t we do not know the values of the partitioning coefficients, `DynRTD` actually contains some more information than `DynWB`. This is also apparent when it is observed that the `DynRTD` systems is connected to the `DynTTD` system, by means of the Niemi's identity (e.g., Niemi (1977)), here written for simplicity only for the transition $\check{L}$:

$$\check{I}(t, t_{in}) = \check{L}(t) p_{\check{L}}(t - t_{in}|t) = \underbrace{\Theta_{\check{L}}(t_{in}) p_{\check{L}}(t - t_{in}|t_{in})}_{\mathcal{F}_{\check{L}}(t,t_{in})} p_{in}(t_{in}) \tag{23}$$

Solving `DynTTD` we know, at any time t the known response $\mathcal{F}_{\check{L}}$ but not the partition function $\Theta_{\check{I}}$. Therefore Equation (23) associates to any backward probability infinitely many forward probabilities compatible with it, each one corresponding to a different value of the partition coefficients $\Theta_{\check{L}}$. Because also $p_L(t - t_[in|t_{in})$ is not known for any time $t' > t$, unless a "ad hoc" assumption is made the backward probabilities alone are not able to determine the forward probabilities future form.

There is an apparent conundrum when considering that there is a one-to-many relation between `DynWB` and `DynTTD` and, for fixed Θs values, a one-to-one relation between `DynTTD` and `DynRTD`. This in fact would imply a one-to-many relation between `DynRTD` and `DynWB`, while it seems to be a one-to-one relation between `DynWB` and `DynRTD`. However, the contraddiction is only apparent since the integration over all the injection times t_i in Eq. (17), to which the response time is subjetc, recollects all the time precipitations together.

5 | THE CONCENTRATION OF A TRACER `DynC`

The fourth dynamical system we are analyzing is the dynamical system that describes the concentrations of a tracer (or a solute or a pollutant), so called $\mathcal{T}$ through the section. According to Figure 1 d) the dictionary of such a system is in Table 10 below.

#	Symbol	Name	Type	Unit
1	E'_{T_S}	$\mathcal{T}$ content in E_T	F	[L T^{-1}]
2	$\hat{L}'$	Percolation of $\mathcal{T}$ from upper storage to lower storage	F	[L T^{-1}]
3	$\check{L}'$	Discharge of $\mathcal{T}$ from the upper reservoir	F	[L T^{-1}]
4	P'	$\mathcal{T}$ in precipitation	F	[L T^{-1}]
5	Q'_l	$\mathcal{T}$ discharge from the lower reservoir	F	[L T^{-1}]
6	Q'_S	$\mathcal{T}$ discharge in surface water	F	[L T^{-1}]
7	R'_l	$\mathcal{T}$ percolation to deeper groundwater	F	[L T^{-1}]
8	S'_l	$\mathcal{T}$ content in the lower storage reservoir	SV	[L]
9	S'_u	$\mathcal{T}$ content in the upper storage	SV	[L]

TABLE 10 Dictionary of `DynC` presented in Figure 1 bottom right.

Table 10 for $\mathcal{T}$ is trivially the analogous of Table 1 for clean water. At this point, we can imagine to work in analogy with what done for water and build all the equation of the $\mathcal{T}$ mass budget, however this is not the way tracers and solutes are treated in literature, where it is usually discussed of their concentration Duffy (2010) and not of their mass and where the knowledge of the water storages and fluxes is used to simplify the solution of the solute system. Therefore for any solute storage S' it is considered its concentration in water, such that:

$$S'(t) := S(t)C(t) \tag{24}$$

where $S(t)$ is the water amount and $C(t)$ the solute concentration. Accordingly we can have for the generic flux $F'(t)$

$$F'(t) := F(t)C_F(t) \tag{25}$$

where $F(t)$ is the water flux and $C_F(t)$ the concentration of the solute in the water flux. As a result, the solute budget equations for upper reservoir of the Kirchner (2016) topology is:

$$\frac{dS_u(t)C_u(t)}{dt} = P(t)C_P(t) - E_{T_S}(t)C_{E_{T_S}}(t) - \check{L}(t)C_{\check{L}}(t) - \hat{L}(t)C_{\hat{L}}(t) \tag{26}$$

where the symbols are explained in the new dictionary for concentrations in Table 11.

#	Symbol	Name	Type	Unit
1	$C_{E_{T_S}}$	$\mathcal{T}$ concentration in E_T	F	[-]
2	$C_{\hat{L}}$	$\mathcal{T}$ concentration in $\hat{L}$	F	[-]
3	$C_{\check{L}}$	$\mathcal{T}$ concentration in $\check{L}$	F	[-]
4	C_P	$\mathcal{T}$ concentration in precipitation	F	[-]
5	C_{Q_l}	$\mathcal{T}$ concentration in Q_l	F	[-]
6	C_{Q_S}	$\mathcal{T}$ concentration in Q_S	F	[-]
7	C_{R_l}	$\mathcal{T}$ concentration in R_l	F	[-]
8	C_{S_l}	$\mathcal{T}$ concentration in S_l	SV	[-]
9	C_{S_u}	$\mathcal{T}$ concentration in S_u	SV	[-]

TABLE 11 Dictionary of concentrations of `DynC`.

A similar equation holds for the lower reservoir:

$$\frac{dS_l(t)C_l(t)}{dt} = \hat{L}(t)C_{\hat{L}}(t) - Q_l(t)C_{Q_l}(t) - R_l(t)C_{R_l}(t) \tag{27}$$

It is then natural that the operator for the places can be set as in Table 12.

#	Symbol	Name	Expression
8	S_l'	T in lower storage	$dS_l(t)C_l(t)/dt$
9	S_u'	T in water in the upper storage	$dS_u(t)C_l(t)/dt$

TABLE 12 Expression for the Water Budget places.

There are several options to solve the above equations, among which we choose the one that allows to establish a connections between the concentrations and the probabilities we have introduced and calculated in the previous sections. According to the standard procedure presented in the supplementary material, the concentration of solute, for instance in the discharge Q_l, can be given as:

$$C_{Q_l}(t) = \int_{-\infty}^{t} p_{Q_l}(t - t_{in}|t)C_{\hat{L}}(t_{in}))dt_{in} := [p_{Q_l} * C_{\hat{L}}](t_{in}) \tag{28}$$

where, on the right end side of the equation we have used the synthetic form for representing the convolution between the probability p_{Q_l} and the initial concentration of $\mathcal{T}$ in that discharge, which is actually the output concentration from the upper reservoir $C_{\hat{L}}(t_{in})$.

The expression table for the solute mass transport is then Table 13 below.

#	Symbol	Name	Expression
1	$C_{E_{T_S}}$	$\mathcal{T}$ concentration in E_T	$[p_{E_{T_S}} * C_P](t_{in})$
2	$C_{\hat{L}}$	$\mathcal{T}$ concentration in $\hat{L}$	$[p_{\hat{L}} * C_P](t_{in})$
3	$C_{\check{L}}$	$\mathcal{T}$ concentration in $\check{L}$	$[p_{\check{L}} * C_P](t_{in})$
4	C_P	$\mathcal{T}$ concentration in P	•
5	C_{Q_l}	$\mathcal{T}$ concentration in Q_l	$[p_{Q_l} * C_{\hat{L}}](t_{in})$
6	C_{Q_S}	$\mathcal{T}$ concentration in Q_S	$C_{\check{L}} + C_{Q_l}$
7	C_{R_l}	$\mathcal{T}$ concentration in R_l	$[p_{R_l} * C_{\hat{L}}](t_{in})$

TABLE 13 The dynamical system `DynRTD` is given trough the assignment of the response time distribution of the fluxes. As explained in the text, these are not giving the same information contained

6 | DISCUSSION AND CONCLUSION

The various HDSys presented in the paper are related and partially alternative ways to face catchment hydrology. `DynWB` is certainly the basic dynamical system, without which the other cannot be solved. From `DynWB` we can obtain any of the other three by applying the functor constructed in the paper and the addition of some information. `DynTTD` is actually obtained by separating the input events globally accounted in `DynWB` but expects that some hypothesis about the water ages sampling, i.e. about the SAS, is made for each one of the compartments present in the system. Recent literature, (e.g., Benettin et al. (2017); van der Velde et al. (2012)), provides hints to identify suitable SAS.

In the paper, however, we fully explored the simplest case of uniform water age sampling, which is actually the case implicitly assumed in most of literature. Niemi's equality is the connection between `DynTTD` and `DynRTD` and allows to obtain one HDSys from the other under some assumptions. `DynRTD`, in fact, assumes that asymptotic partition coefficients, the Θs, are known, which is usually not known for any finite time. At time t, the complete equivalence is not between backward pdf and life expectation pdf but between backward pdf and the known responses, $\mathcal{F}$. However, in practice, it can be found an effective concentration time, $t_c(t)$, after which the $\Theta(t_{in})$ variations are negligible. The `DynC` by definition introduces new substances and therefore new requirements. It turns out that for passive solutes the only further information needed is the concentration of the substance in the input.

One additional note has to be done on how what presented in this paper makes easier the computation. Computation usually is built upon tables as those presented in the supplemental material and in Benettin and Bertuzzo (2018), whose columns are the injection times, the rows the current time (for places) or the exit time for transitions, and the entries are, respectively, the quantity of water inside the place and the quantity of water exiting with a given flux. Maintaining one of such tables for any place and transition allows the determination of any of the probabilities introduced in this paper with simple operations, either they derive from measurements or from computation. The concentrations, cause the relation exploited in this paper, simply follow from the multiplication of these tables entries by the solute/tracers concentration in input and their accounting does not need any further equation solving.

To summarize, in this paper we discussed the relations of various hydrological dynamical systems, i.e., the dynamical systems of backward travel times distribution, of response time distribution and of concentrations, starting from the water budget. What we wanted to show is the following:

- given the topology of those dynamical systems, then the writing of equations easily follows;
- the equations of the different dynamical systems have a legacy;
- moving from one HDSys to the others, some information as has to be acquired or some assumption to be made: about the SAS for getting `DynTTD` from `DynWB`; about Θs when going from `DynTTD` to `DynRTD`; about initial solute/tracers inputs for getting the `DynC`.
- After the assumptions are made, all the quantities can be easily estimated

acknowledgements

The paper has been partially supported by the PRIN 2017 project WATZON.

conflict of interest

The authors declare that they have no conflict of interest.

Data Availability Statement

The authors declare that they don't have used data in the paper.

A | SUMMARY OF EXTENDED PETRI NETS CHARACTERISTICS

EPN are a mathematical modelling language for the description of the hydrological dynamical systems (`HDSys`). They standardize the way `HDSys` are represented and facilitate the user comprehension of all the possible eco-hydrological

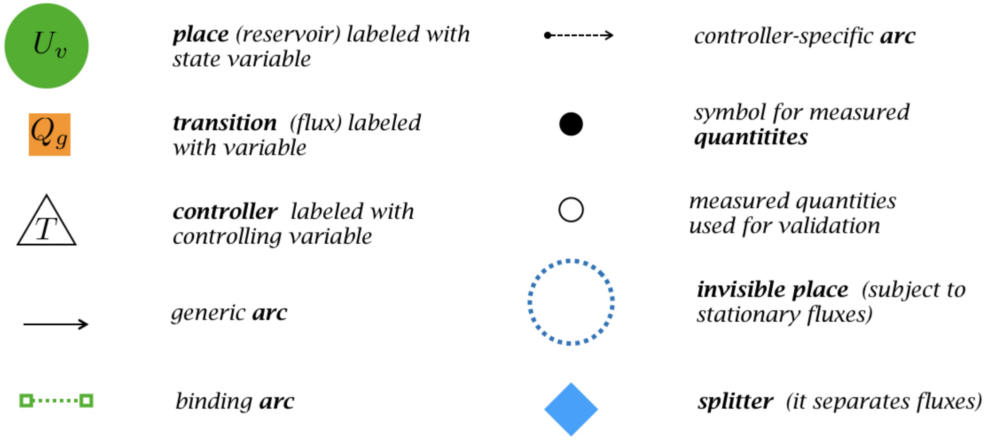

FIGURE 2 Principal objects in the extended Petri Nets representation.

interactions. In the following, a brief summary of the important concepts of the EPN, extracted from Bancheri et al. (2019), is reported.

Figure 2 shows the principal graphical objects in EPN:

- reservoirs (called places) are represented as circles;
- fluxes (called transitions) between reservoirs (or places) are represented as squares;
- controllers, which are quantities in charge of regulating fluxes, are represented as triangles;
- connections between places and transitions are represented as generic arc;
- binding arcs are used when two different fluxes in two different budgets contain the same variable;
- connections from places to controllers and from controllers to transition are represented as oriented dashed arcs;
- small, solid, black circles are used to mark measured quantities, i.e. the climatic variables;
- small, empty circles represent quantities that are also given but are used to assess the goodness of the model, i.e. discharge measurements against which the model is calibrated;
- big circles with dotted borders represent hidden places, whose budget is stationary;
- splitters represent partition coefficients, i.e. when transition are connected to more than one place.

To complete the information, two other elements should be added:

- a dictionary giving the names of the symbols in the graphic, conveying their meaning;
- an expression table giving mathematical completeness to the fluxes.

Applying the rules previously introduced, it is easy to cast any model into the EPN representation, as it is clearly shown in Bancheri et al. (2019), where three examples are reported.

EPN facilitates the construction of the appropriate numerical model of a catchment from the experimental evidence in the "perceptual phase" of research. Moreover, thanks to their compositional property, they allow to represent a single hydrological response unit as well as a complex catchment, where multiple systems of equations are solved simultaneously.

Finally, EPN can be used to describe complex earth system models that include feedback between the water, energy and carbon budgets. The representation of `HDSys` with EPN provides a clear visualization of the relations and feedback between subsystems, which can be studied with techniques introduced in contemporary non-linear systems theory and control theory.

references

Bancheri, M., Serafin, F. and Rigon, R. (2019) The representation of hydrological dynamical systems using the extended petri nets. *Water Resources Research*, **8 (01)**, 159–27.

Benettin, P. and Bertuzzo, E. (2018) tran-sas v1. 0: a numerical model to compute catchment-scale hydrologic transport using storage selection functions. *Geoscientific Model Development*, **11**, 1627–1639.

Benettin, P., Soulsby, C., Birkel, C., Tetzlaff, D., , G. and Rinaldo, A. (2017) Using sas functions and high resolution isotope data to unravel travel time distributions in headwater catchments. *Water Resources Research*, **53**, 1864–1878. URL: http://doi.org/10.1002/2016WR020117.

Beven, K. J. (2011) *Rainfall-runoff modelling: the primer*. John Wiley & Sons.

Botter, G., Bertuzzo, E. and Rinaldo, A. (2010) Transport in the hydrologic response: Travel time distributions, soil moisture dynamics, and the old water paradox. *Water Resources Research*, **46**, W03514. URL: http://doi.org/10.1029/2009WR008371.

— (2011) Catchment residence and travel time distributions: The master equation. *Geophysical Research Letters*, **38**.

Bradley, T.-D. (2018) What is applied category theory?

Calabrese, S. and Porporato, A. (2015) Linking age, survival, and transit time distributions. *Water Resources Research*, **51**, 8316–8330. URL: http://doi.org/10.1002/2015WR017785.

Duffy, C. (2010) Dynamical modelling of concentration-age-discharge in watersheds. *Hydrological Processes*, **24**, 1711–1718. URL: http://doi.org/10.1002/hyp.7691.

Fong, B. and Spivak, D. (2018) Seven scketches in compositionality: an invitation to theory. *arXic:math.CT*.

Gabrielli, C. P., Morgenstern, U., Stewart, M. K. and Mcdonnell, J. J. (2018) Contrasting groundwater and streamflow ages at the maimai watershed. *Water Resources Research*, **54**, 3937–3957. URL: http://doi.org/10.1029/2017WR021825.

Gupta, V. K. and Waymire, E. (1983) On the formulation of an analytical approach to hydrologic response and similarity at the basin scale. *Journal of Hydrology*, **65**, 95–123.

Kirchner, J. (2016) Aggregation in environmental systems -partÂ 2: Catchment mean transit times and young water fractions under hydrologic nonstationarity. *Hydrology and Earth System Sciences*, **20**, 299–328. URL: http://doi.org/10.5194/hess-20-299-2016.

— (2019) Quantifying new water fractions and transit time distributions using ensemble hydrograph separation: theory and benchmark tests. *Hydrol. Earth Syst. Sci.*, **23**, 303–349. URL: https://doi.org/10.5194/hess-2018-429.

Maloszewski, P. and Zuber, A. (1982) Determining the turnover time of groundwater systems with the aid of environmental tracers. *Jour. Hydrol.*, **57**, 207–231.

McGuire, K. and McDonnell, J. (2006) A review and evaluation of catchment transit time modeling. *Journal of Hydrology*, **330**, 543–563.

Niemi, A. J. (1977) Residence time distribution of various flow processes. *International Journal of Radiation and Isotopes*, **28**, 855–860.

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

Rigon, R., Bancheri, M. and Green, T. R. (2016b) Age-ranked hydrological budgets and a travel time description of catchment hydrology. *Hydrology and Earth System Sciences*, **20**, 4929.

Rihel, E. (2016) *Category theory in context*. Dover.

Rodríguez-Iturbe, I. and Rinaldo, A. (2001) *Fractal river basins: chance and self-organization*. Cambridge University Press.

Rodríguez-Iturbe, I. and Valdes, J. B. (1979) The geomorphologic structure of hydrologic response. *Water resources research*, **15**, 1409–1420.

Sprenger, M., Stumpp, C., Weiler, M., Aeschbach, W., ST, A., Benettin, P., Dubbert, M., Hartmann, A., Hrachowitz, M., Kirchner, J., McDonnel, J., Orlowski, N., Penna, D., Pfahl, S., Rinderer, M., Rodriguez, N., Schmidt, M. and Werner, C. (2019) The demographics of water: A review of water ages in the critical zone. *Rev. Geophys.*, **2018RG000633**.

van der Velde, Y., Torfs, P., van der Zee, S. and Uijlenhoet, R. (2012) Quantifying catchment-scale mixing and its effect on time-varying travel time distributions.