A virtual tracer experiment to assess the temporal origin of root water uptake, evaporation, and drainage

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Abstract
The temporal origin of drainage, evaporation, and root water uptake (RWU) are indicators of ecosystem functioning that shed light on how natural and anthropogenic disturbances affect plant resilience and aquifer vulnerability. A virtual tracer experiment was carried out in HYDRUS-1D using data from a soil lysimeter planted with winter rye in Austria. The RWU ($t_R$), evaporation ($t_E$), and drainage ($t_D$) transit times ($t$) were determined by using the actual dispersivity optimized in a prior study. First, $t_R$ and $t_D$ were compared to RWU ($t_{PT,R}$) and drainage ($t_{PT,D}$) advective transit times estimated using the particle tracking algorithm. The $t_R$ values were in agreement with $t_{PT,R}$ while large discrepancies were detected when estimating drainage transit times using the two approaches. A sensitivity analysis revealed that dispersivity had a mild, poor, and strong influence on $t_R$, $t_E$, and $t_D$. The longitudinal dispersivity describes how a tracer spreads along the flow paths. The longer the flow paths, the more dispersion affects the tracer transport. On average, water parcels originating from rainfall in the growing season took 18 and 201 days to reach the roots (with RWU being 21% of rainwater) and the soil profile bottom (with drainage being 36% of rainwater), respectively. In contrast, 10% of rainwater that fell in the dormant season became RWU after 264 days, while 79% became drainage after 294 days. The temporal origin of water can be explored in other plots by using the guidelines proposed in this study.

KEYWORDS
HYDRUS-1D, lysimeter, particle tracking, tracer mass balance, transit time distribution (TTD), water-stable isotopes

1 | INTRODUCTION

Optimal management of terrestrial (agricultural, urban, and forest) ecosystems relies on water balance simulations using process-oriented hydrological models. Such modelling tools require a large amount of environmental input data, which can only be retrieved from modern monitoring infrastructures and intensive sampling campaigns (Romano et al., 2018; Vereecken et al., 2015; Yang et al., 2021). Still, the hydrological processes need to be better understood to develop sustainable policies under rapid climate and land use changes. A critical component of hydrologic sensitivity to external forcings and plant characteristics arises from changes in the timing of water delivery to the soil–plant-atmosphere continuum (SPAC). Knowledge of the temporal origin of drainage ($D$), evaporation ($E$), and root water uptake ($RWU$) helps understand the impact of natural and anthropogenic disturbances, such as drought and transport of contaminants to groundwater, on plant resilience and aquifer vulnerability (Sousa et al., 2013; Sprenger et al., 2019). An important variable for defining the water's
Field tracer experiments are used to assess the arrival time at the target position of a tracer injected at the entry position and transported across the porous medium by advection and hydrodynamic dispersion. The arrival time is usually estimated at the peak tracer concentration from the target point (Sprenger et al., 2016). Virtual tracer experiments help track water pathways across the SPAC originating from a long sequence of rainfall events and are used to assess the temporal origin of RWU and drainage. Yet the implementation of virtual tracer experiments is not straightforward, and clear guidelines are still missing in the literature (Asadollahi et al., 2020; Brinkmann et al., 2018; Haverd & Cuntz, 2010; Sprenger et al., 2016).

In this study, a special isotope-enabled module of HYDRUS-1D (Huang et al., 2015; Šimůnek et al., 2016; Sprenger et al., 2015; Stumpf et al., 2012) was used for simulating water flow and tracer transport for five years in a soil lysimeter planted with winter rye in Austria (Stumpf et al., 2012). This isotope-enabled module assumes that the advection-dispersion equation governs the tracer transport in soils and allows tracers to leave the soil profile with evaporation (contrary to other types of solutes). Still, the tracer transport simulation is influenced by the hydrodynamic dispersion, $\lambda$ (either measured, calibrated, or commonly assumed as 1/10th of soil profile depth), and the transit time is not given directly as a model output.

By contrast, particle tracking is a well-established approach to assess advective transit time in many modelling applications over different spatial and temporal scales (Baek & Lee, 1996; Bechtold et al., 2011; Danesh-Yazdi et al., 2018; de Rooij et al., 2013; Wlusz et al., 2019). The particle tracking algorithm was recently implemented in version 5 of HYDRUS-1D to trace water pathways in the soil profile from which RWU and drainage transit times are estimated (Zhou et al., 2021; Zhou et al., 2022).

Few studies have attempted to assess the temporal origin of RWU, evaporation, and drainage using HYDRUS-1D for experimental lysimeters or soil profiles (Asadollahi et al., 2020; Brinkmann et al., 2018; Sprenger et al., 2016). To our knowledge, the virtual tracer experiment has not yet been evaluated with a particle tracking algorithm, and the impact of dispersivity on transit time is mostly unexplored. Asadollahi et al. (2020) used a tracer tracking approach to estimate the age of evapotranspiration and drainage for two experimental lysimeters containing 200 cm-thick layered soil columns. The above authors set evaporation to zero and assumed potential transpiration equal to potential evapotranspiration. If water can leave the system only through root water uptake by neglecting evaporation, the resulting water transit times of evapotranspiration may be biased versus older ages (otherwise, younger water would be allowed to leave the soil via evaporation). Sprenger et al. (2016) and Brinkmann et al. (2018) used the isotope-enabled module of HYDRUS-1D to simulate isotope transport in the critical zone. Sprenger et al. (2016) used the virtual tracer experiment to assess RWU and drainage transit time distribution over thirty-five 200-cm-thick layered soil profiles and determined the rainfall contribution to RWU and drainage but neglected evaporation. The temporal origin of water taken up by Fagus sylvatica and Picea abies was determined by using 4-year-long isotope transport simulations in two 70-cm-thick soil profiles (Brinkmann et al., 2018), combining RWU patterns with soil water residence time distributions at different soil depths to estimate age distributions of RWU. Brinkmann et al. (2018) missed to assess the drainage and evaporation transit time and rainfall partitioning into evaporation, transpiration, and drainage.

The main research questions are:

i. What are the differences in RWU and drainage transit times when using the particle tracking approach (advective transport) and the virtual tracer experiment (advective and dispersive transport)?

ii. What is the impact of dispersivity on tracer transport in the virtual tracer experiment?

iii. How to assess the temporal origin of evaporation, transpiration, and drainage in the virtual tracer experiment?

These research questions were addressed in three steps (Figure 1). First, the advective RWU and drainage transit times ($\tau_{PT,R}$ and $\tau_{PT,D}$) were obtained from particle tracking and compared to the advective-dispersive transit times ($\tau_{R}$ and $\tau_{D}$) obtained from the virtual tracer experiment (red box in Figure 1). Second, the sensitivity analysis was carried out to evaluate the effect of dispersivity on the tracer transport simulations and estimations of RWU, evaporation, and drainage.
drainage transit times (green box in Figure 1). Third, the tracer-based
transit times and contributions of rainwater to evaporation, transpiration,
and drainage were calculated and aggregated at selected temporal resolutions (blue box in Figure 1).

2 | MATERIALS AND METHODS

2.1 | Site description and data availability

The datasets used in the present paper are taken from Stumpp et al. (2012), who described a lysimeter experiment carried out at the experimental site located at the research area of the HBLFA Raumberg-Gumpenstein, 190 km southwest of Vienna (Austria). This region is characterized by a temperate climate with a mean annual temperature of 6.9°C and mean annual precipitation of 1035 mm. A total of five 150-cm-thick lysimeters (Lys1-Lys5) with a surface area of 1 m² were installed in agricultural fields that differed in their crop and fertilization methods. This study considers the third lysimeter (Lys3) containing a layered soil monolith planted with winter rye (Secale cereale L.), sown each October, and harvested by the end of August. Leaf area index (LAI) and rooting depth were determined daily, ranging between 0 and 2.9 m² m⁻² and 0 and 100 cm, respectively; here, maximum values were provided by onsite operators and from the literature (Allen, 2000; Bohner et al., 2007; Knisel & Davis, 2000) as given in detail in Stumpp et al. (2012). The soil profile is made up of three soil layers (−30 cm < z < 0 cm, −90 cm < z < −30 cm, −150 cm < z < −90 cm). For the period between May 2002 and February 2007, daily values of precipitation and crop-specific potential evapotranspiration (ETₚ) are available.

2.2 | HYDRUS-1D model setup

In this study, we used version 5 of HYDRUS-1D (Simunek et al., 2016; Stumpp et al., 2012), and data available in the project Lys3_Stumpp, which can be downloaded from the HYDRUS website (https://www.pc-progress.com/en/Default.aspx?h1d-lib-Isotope).

The simulation period is 1736 days, from 3rd May 2002 to 1st February 2007 (corresponding to almost five years). The 150-cm-thick soil profile is composed of three soil layers (−30 cm < z < 0 cm, −90 cm < z < −30 cm, −150 cm < z < −90 cm). The van Genuchten (1980) parameters (θᵣ, θₛ, α, n, Kₛ, l) of the soil water retention and hydraulic conductivity functions (Table 1) were calibrated by Stumpp et al. (2012) to provide physically-based descriptions of soil water content and pressure head values in each soil layer and drainage fluxes (Data S1).

The potential water flux across the soil surface (r_top), defined as the difference between daily values of potential evaporation (E_p) and precipitation (P), was used as the upper boundary condition for water flow. The lower boundary condition was set to a seepage face by imposing a zero pressure head (ψ = 0 cm) when the soil profile bottom was saturated and a zero water flux when it was unsaturated. The actual water flux (drainage, D) across the soil profile bottom is referred to as V_d.

Crop-specific potential evapotranspiration (ETₚ) is partitioned into potential evaporation (Eₚ) and transpiration (Tₚ), which, when distributed over the root zone, gives potential RWU using the following empirical equation (Ritchie, 1972):

\[ E_p = ET_p e^{-k \cdot LAI} \]  

where k (−) is the dimensionless extinction coefficient for global solar radiation inside the canopy. The LAI was measured (Section 2.1), while k was assumed to be equal to 0.6 (Stumpp et al., 2012). The residual fraction of ETₚ was assumed to be equal to Tₚ. The root water extraction rate occurs through the roots distributed across the root zone according to a piece-wise function proposed by Hoffman and van Genuchten (1983). The roots extend from the soil surface to the bottom of the root zone with the maximum and minimum root density, respectively. The rooting depth is time-variant during the growing season, and the maximum rooting depth is set to be equal to 100 cm. Actual RWU is obtained as a product of potential RWU (or Tₚ distributed over the root zone) and the stress response function, a piecewise linear reduction function proposed by Feddes et al. (1978). The so-called Feddes stress response function depends on prescribed pressure head values. The default values in Hydrus-1D for wheat were used in our calculations. Crop uptake is reduced below ψ = −500 or −900 cm depending on whether the potential transpiration rate is high or low, respectively. The matric pressure head at the wilting point corresponds to ψ = −16 000 cm. The actual surface flux (w_top) is given as the difference between actual evaporation (Eₚ) and precipitation (P) and depends on limiting pressure heads on the soil surface. Details about the model setup for water flow are reported in Table A1 and Data S1.

2.3 | Assessing RWU and drainage transit time with particle tracking

The particle tracking algorithm, recently implemented in HYDRUS-1D (Zhou et al., 2021), requires the following two input parameters: w_Init and w_Prec. The w_Init parameter represents the initial water storage between particles and determines the particle positions along the soil

<table>
<thead>
<tr>
<th>Profile interval</th>
<th>θᵣ</th>
<th>θₛ</th>
<th>α</th>
<th>n</th>
<th>Kₛ</th>
<th>l</th>
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<tr>
<td>−30 &lt; z &lt; 0</td>
<td>0.00</td>
<td>0.30</td>
<td>0.023</td>
<td>1.14</td>
<td>110</td>
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<tr>
<td>−90 &lt; z &lt; −30</td>
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<td>0.32</td>
<td>0.076</td>
<td>1.07</td>
<td>600</td>
<td>0.5</td>
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<tr>
<td>−150 &lt; z &lt; −90</td>
<td>0.00</td>
<td>0.32</td>
<td>0.016</td>
<td>1.90</td>
<td>110</td>
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depth at the initial time, $t_0$. The $w_{\text{prec}}$ parameter is the amount of water that passes through the soil surface before a new particle is released. This means that particles are released at the soil surface only under humid conditions, that is, when infiltration exceeds actual evaporation. Under dry conditions, the surface flux is directed out of the soil profile; thus, new particles are not released. Instead, existing particles may exit from the soil surface due to evaporation. By setting $w_{\text{prec}} = -1$, a new particle is launched whenever the actual surface flux becomes negative ($v_{\text{Top}} < 0$), that is, when precipitation exceeds actual evaporation. The particle tracking algorithm considers only convective transport and neglects dispersion. See details in Data S1.

Figure 2 depicts an illustrative example for estimating drainage ($t_{\text{PT,D}}$) and RWU ($t_{\text{PT,R}}$) advective transit times using the particle tracking algorithm (Figure 2a). By selecting the third precipitation event (green bar in Figure 2a) at entry time ($t_{\text{in}}$), the corresponding particle trajectory across the soil profile (extracted from the output text file “Particles.out”, which contains the z-coordinates of particle positions over time) is depicted by the black line (Figure 2b). The arrival time at the target point ($t_{\text{out}}$) is identified as the time when the particle exits from the soil profile bottom (Figure 2b). The output file “Uptake.out” contains the root water uptake flux fed by the tracked water parcel. The arrival time of RWU is considered the time when the cumulative actual RWU reaches its maximum value. A transit time distribution is obtained by analysing the advective transit times of all particles released at the soil surface. An open-access Matlab script (PT.m) is shared to read the output text files (more details are provided in Data S1).

2.4 Assessing RWU, evaporation, and drainage transit time and rainfall partitioning with the virtual tracer experiment

The isotope-enabled module in HYDRUS-1D accounts for isotope transport so that isotopes (or tracers) do not accumulate at the soil surface and leave the soil profile with the evaporation flux (Stumpf et al., 2012). Evaporation fractionation is not considered in the virtual tracer experiment.

The initial tracer concentration was set to zero in the entire soil profile. Roots can take up the tracer with unlimited passive root tracer uptake by setting the $c_{\text{Root max}}$ parameter to a large value. The actual tracer flux across the soil surface and soil profile bottom are denoted as $c_{\text{VTop}}$ and $c_{\text{VRoot}}$, respectively, while the actual root tracer uptake in the root zone is called $c_{\text{VRoot}}$. Ten observation points were inserted at the following soil depths: $z = -5, -15, -30, -45, -60, -75, -90, -105, -120, \text{and} -135 \text{ cm}$.

The number of simulations in the virtual tracer experiment depends on the total number of daily precipitation events (Nasta et al., 2023). In each ith simulation, a hypothetical tracer concentration is injected with the ith precipitation event by keeping the $c_{\text{Top}}$ values of the other rainfall events equal to zero. A zero concentration gradient (free drainage) is used as the lower boundary condition.

Thirteen rainfall events are shown in the illustrative example of Figure 3, and the tracer is injected with the third labelled rainfall event (cyan bar in Figure 3a). The main steps related to the tracer transport simulation to obtain the drainage ($t_{\text{D}}$) and RWU ($t_{\text{R}}$) transit times and rainfall partitioning are:

1. To fix an arbitrary tracer concentration (i.e., $c_{\text{Top}} = 100$) in the labelled rainfall event; for instance, the input tracer flux, $c_{\text{VTop}} = -100$ if $v_{\text{Top}} = -1.0 \text{ cm d}^{-1}$ (cyan bar in Figure 3a);
2. To obtain the output tracer flux across the soil profile bottom, $c_{\text{VBot}}$ (Figure 3b), and the root system, $c_{\text{VRoot}}$ (Figure 3c); the arrival time ($t_{\text{Arr}}$) is defined as the time of median breakthrough curve (Isch et al., 2022; Nasta et al., 2023; Sprenger et al., 2016) and the rainfall contribution to water balance components is the ratio...
Assessing RWU and drainage transit time with particle tracking

A total of 803 precipitation events entering the soil surface \( (v_{\text{top}} < 0) \) were identified. The water parcels of 167 active rainfall events reached the bottom of the soil profile. The remaining water parcels returned to the atmosphere via evapotranspiration. Figure 4 shows the particle trajectories (coloured lines in Figure 4b) originating from the 167 active rainfall events and actual fluxes at the upper \( (v_{\text{top}}) \) blue line in Figure 4a) and lower \( (v_{\text{bot}}) \) green line in Figure 4c) boundaries. Note that the last 18 particle pathways were not included among the 167 events because they did not reach the soil profile bottom within the simulation time. Estimating the drainage transit times associated with the 167 rainfall events was straightforward by tracking the particle positions in the soil profile. Several water parcels were tracked within the root zone (black line in Figure 4b) for a time period during the growing season. This range of time is defined as the root zone soil water residence time, which refers to the age of a water parcel travelling within the root system. By contrast, the (expressed in % of rain becoming \( E_a, T_a, \) and D) between the output and the input tracer fluxes. The output tracer flux is associated with actual evaporation, actual RWU (transpiration), or drainage, whereas the input tracer flux is associated with the rainfall. More details are reported in Data S1.

The active precipitation events (the term “active” refers to those events which were able to reach the bottom of the soil profile) identified by the particle tracking algorithm (Section 3.1) were simulated using the virtual tracer approach (Section 3.2) to ensure a fair comparison of results in the first subset of virtual tracer experiments (red box in Figure 1). Two levels of dispersion were considered by using: (i) the originally calibrated dispersivity \( (\lambda_a = 4.7 \text{ cm}) \) and (ii) the minimum dispersivity \( (\lambda_a = 0.5 \text{ cm}) \) not causing numerical instability problems. The latter allowed a consistent comparison with particle tracking (advection-dominated transport) results to minimize the impact of dispersivity on the estimated transit times in the virtual tracer experiment while maintaining the Peclét stability criterion. We calculated the root mean square error (RMSE) between \( \tau_D \) and \( \tau_R \) and the corresponding \( \tau_{PT,D} \) and \( \tau_{PT,R} \) (Section 3.2).

Another set of rainfall events was used to carry out a sensitivity analysis to evaluate the impact of \( \lambda_a \) on the tracer transport simulations and the estimation of RWU \( (\tau_R) \), evaporation \( (\tau_E) \), and drainage \( (\tau_D) \) transit times (green box in Figure 1). The mean error (ME) was calculated between reference \( \tau_R, \tau_E, \) and \( \tau_D \) obtained by using the original dispersivity \( (\lambda_a = 4.7 \text{ cm}) \) and \( \tau_R, \tau_E, \) and \( \tau_D \) obtained by using a range of \( \lambda_a \) values between 0.5 cm and 20 cm (Section 3.3).

Finally, the virtual tracer experiment was carried out to assess the rainfall contributions to RWU, evaporation, drainage, and associated transit times by keeping the actual dispersivity (blue box in Figure 1). We selected only the effective rainfall events \( (P > E_a) \) to ensure negative (downward) \( \tau_{PT,D} \) values (Section 3.4). Transit times and rainfall partitioning based on tracer transport simulations were aggregated on a seasonal basis. Two seasons were identified in this study: growing and dormant season. The growing season lasts from May to August (when LAI and root depth values are above zero), and the dormant season from September to April (when LAI and root depth values are zero). This means that we tracked the precipitation events from May to August (the growing season’s precipitation) or from September to April (the dormant season’s precipitation) to see whether they were used during the vegetation period for transpiration.

An open-access Matlab script (VTE.m) is shared to automate the virtual tracer experiment simulations (more details are provided in Table A1 and Data S1).
RWU transit time was defined as the water age leaving the soil system through the roots across the soil profile.

Figure 5 shows the frequency distributions of drainage and RWU advective transit times of the 167 rainfall events obtained using particle tracking. Normality tests (Lilliefors and Kolmogorov–Smirnov executed in Matlab) rejected the null hypothesis that the statistical distributions of the advective transit time values (drainage transit time, \( \tau_{PT,D} \), in Figure 5a, and RWU transit time, \( \tau_{PT,R} \), in Figure 5b) are normal at the 5% significance level. Therefore, the median (309.9 days for \( \tau_{PT,D} \) and 208.9 days for \( \tau_{PT,R} \)) and mode (334.5 days for \( \tau_{PT,D} \) and 234.7 days for \( \tau_{PT,R} \)) values were reported instead of the mean values (296.1 days for \( \tau_{PT,D} \) and 191.7 days for \( \tau_{PT,R} \)). A few events on the right tail of Figure 5a influenced the drainage transit time distribution, while the RWU transit time distribution was skewed by low values (Figure 5b), indicating that roots took up most rainfall water during the growing season. This was partially caused by the rooting depth of winter rye being shallow during early growing seasons, resulting in short RWU transit times (Figure 5b).

### 3.2 Comparing particle tracking and virtual tracer experiment

The active 167 precipitation events identified by the particle tracking algorithm were simulated using the virtual tracer experiment.

Figure 6 shows the comparison between advective transit times (\( \tau_{PT,D} \) and \( \tau_{PT,R} \)) obtained using particle tracking and those (\( \tau_D \) and \( \tau_R \)) obtained using particle tracking and tracer transport modeling. The root mean square error (RMSE) values are reported in each subplot.
using the virtual tracer experiment. The corresponding model performance was evaluated in terms of RMSE values. The transit time based on the virtual tracer experiment was identified by fixing dispersivity to the original value (λ_L = 4.7 cm) calibrated in Stumpf et al. (2012) and to the minimum value (λ_L = 0.5 cm). Figure 6a shows that many τ_D values based on λ_L = 4.7 cm are smaller than the corresponding advective drainage transit times (red circles) with a relatively large difference (RMSE is about 50 days). The τ_R values based on λ_L = 4.7 cm and the RWU advective transit time (green circles in Figure 6b) aligned fairly well, especially for values above 160 days, with an RMSE of about 21 days. The lowest τ_R values were below the identity line.

By minimizing the impact of hydrodynamic dispersion (λ_L = 0.5 cm) on the tracer transport simulations, the drainage transit times (magenta circles in Figure 6c) aligned well on the 1:1 line with few exceptions due to numerical instabilities. The RMSE values decreased substantially to estimate drainage transit time when the longitudinal dispersivity was reduced to λ_L = 0.5 cm. The RWU transit times (yellow circles in Figure 6d) did not change much when setting λ_L = 0.5 cm. The longitudinal dispersivity describes the spreading of a tracer along the flow paths. The longer the flow paths, the more affected by dispersion the tracer transport is; thus, drainage transit times are very sensitive to λ_L. The root zone is denser near the soil surface, that is, at the beginning of the flow paths, and therefore, the effect of dispersion on RWU is less pronounced.

### 3.3 Sensitivity analysis to evaluate the impact of dispersivity on tracer-based transit time

Dispersivity is a transport parameter describing the spreading of a solute or tracer. Dispersivity controls the shape of the breakthrough curve and therefore influences the arrival time estimation. In a new model simulation set, we considered 370 rainfall events in the virtual tracer experiment. Figure 7 shows the sensitivity analysis to evaluate the impact of λ_L on the transit times (τ_R, τ_E, and τ_D) in terms of the mean error (ME) between the transit time based on the actual λ_L and those based on λ_L ranging from 0.5 and 20 cm. As expected, λ_L influences transit times differently. If λ_L becomes smaller or greater than the original dispersivity (λ_L = 4.7 cm), the RWU and evaporation (red and grey curves in Figure 7) transit times moderately decrease or increase, respectively. Dispersivity has a higher impact on drainage transit time, leading to a significant rise in inaccuracy as dispersivity increases (blue curve in Figure 7). If dispersivity is almost null (λ_L = 0.5 cm), ME of τ_R, τ_E, and τ_D is 0.90, 10.1, and –18.4 days, respectively. When dispersivity is unknown, several authors arbitrarily fix it at 1/10th of the travel distance as a rule of thumb (Gelhar et al., 1992; Nasta et al., 2021; Sprenger, Tetzlaff, Buttle, Laudon, & Soulsby, 2018; Vanderbooght & Vereecken, 2007). This assumption (λ_L = 15.0 cm = 1/10th of the 150-cm-thick soil profile) led to ME of τ_R, τ_E, and τ_D of –2.4, –7.9, and +32.4 days. The deviation from the reference situation deteriorates substantially for the estimation of τ_D (ME = +43.1 days) and moderately for the estimation of τ_R (ME = −2.7 days) and τ_E (ME = −10.3 days), when λ_L = 20 cm.

### 3.4 Assessing the temporal origin of RWU, evaporation, and drainage

The subset 370 model simulations carried out in Section 3.3 was used in this Section to assess the temporal origin of the main water balance components. Event-based transit times (and corresponding breakthrough curves) and rainfall contributions to actual evaporation, actual transpiration, and drainage are illustrated in Figure 8. Drainage and actual evaporation are the dominant hydrological fluxes in the study area, as illustrated in Figure 8a,b (Figure S1 in Data S1). The cumulative tracer drainage fluxes (blue curves in Figure 8d) indicate a migration time of the tracer between 115 and 454 days from the soil surface to the soil profile bottom. Low drainage transit times are induced by frequent and intensive rainfall events following the selected labelled rainfall event, pushing the tracked water parcel quickly downward towards the soil profile bottom. By contrast, a dry period after the selected rainfall event causes a slow migration of the water parcel across the soil profile. The vast majority of evaporation fluxes are lost within the first ten days (Figure 8e), with a few cumulative tracer evaporation fluxes (grey curves in Figure 8f) characterized by a delay of 50–120 days. RWU transit times range from 2 to 358 days (Figure 8g) resulting from the corresponding root tracer fluxes (red curves in Figure 8h). High RWU ages are associated to low RWU rates and vice versa. On the one hand, the old water parcels travel for a few days within the deepest portion of the root zone, where roots have the minimum density. On the other hand, the young water parcels reside in the uppermost portion of the root zone and are subject to the highest rates of RWU. The frequency distributions of RWU, evaporation, and drainage transit times (not shown) are not normal according to the normality tests (Lilliefors and Kolmogorov–Smirnov executed in Matlab) mentioned in Section 3.1. The distributions of drainage and RWU transit times are multimodal, while the evaporation transit time distribution is exponential, with few values surpassing ten days.

The 370 RWU, evaporation, and drainage transit time values were grouped into precipitation sources from two seasons (growing and
dormant seasons). On average, it took 18, 3, and 201 days for rainfall water in the growing season to reach the roots (with actual RWU being 21% of rainwater), the soil surface (with actual evaporation being 42% of rainwater), and the soil profile bottom (with drainage being 36% of rainwater), respectively. In contrast, 10%, 10%, and 79% of rainfall from the dormant season reached the roots, the soil surface, and the soil profile bottom after 264, 6, and 294 days, respectively.

Most water parcels originating from the rainfall of the growing season were quickly removed by dominant evapotranspiration fluxes. Nevertheless, the cumulative root tracer fluxes were grouped into two distinct sets for precipitation from the growing and dormant seasons (separation of RWU tracer breakthrough curves according to seasons is given in Figure S2 in Data S1). The histogram for precipitation from the growing season provides an exponential RWU transit time distribution with the majority of arrival times below 15 days. The RWU transit time multimodal distributions from the dormant season’s precipitation had two peaks at 81 and 298 days (Figure S2). The longest RWU transit times (>200 days) originated from waters infiltrating at the beginning of the previous dormant season. The grouping of evaporation and drainage transit time distributions did not provide two distinct sub-distributions (not shown).

4 | DISCUSSION

4.1 | The virtual tracer experiment for assessing the temporal origin of RWU, evaporation, and drainage

Several factors, including the depth and the soil hydraulic properties of each layer, the time-variant crop characteristics, the seasonal pattern of the atmospheric forcings, and the hydrodynamic dispersion, influence the assessment of the transit time through the vadose zone. Stumpp et al. (2012) measured or calibrated all these factors.

**FIGURE 8** (a) Rainfall contribution (in %) to actual evaporation, $E_a$ (grey), actual transpiration, $T_s$ (red), and drainage, $D$ (blue) for the 370 rainfall events, (b) a pie chart of rainfall partitioning resulting from the tracer mass balance, (c) drainage transit times ($\tau_D$) and (d) corresponding cumulative bottom tracer fluxes ($cv_{Bot}$), (e) evaporation transit times ($\tau_E$) and (f) the corresponding cumulative surface tracer flux ($cv_{Top}$), (g) RWU transit times ($\tau_R$) and (h) the corresponding cumulative root tracer flux ($cv_{Root}$). The vertical dashed lines delimit the precipitation events from growing (GS) and dormant (DS) seasons (subplots a, c, e, g).
In this study, we assessed the age dynamics of water in a 150-cm-thick layered soil profile beneath winter rye. Importantly, setting the arrival time when the trace breakthrough is 50% reflects the definition of median time provided by Benettin et al. (2015), who envision the existence of a time distribution associated with the output tracer flux originating from each rainfall event. The arrival times estimated using tracer transport simulations were compared to those estimated using the particle tracking algorithm. Both methods need to be validated with field tracer experiments. The median (309.9 days), mode (334.5 days), and mean (296.1 days) of advective $\tau_{PT,D}$ are reported above in Section 3.1. The tracer-based approach resulted in the median, mode, and mean of $\tau_D$ of 262.0, 308.5, and 260.5 days, respectively. Stumpp et al. (2012) calculated the mean drainage transit time by considering the shift in the isotope peaks between input and output on the soil surface and lysimeter bottom while correcting the peak time by accounting for the given dispersivity. The mean drainage transit time in the third lysimeter (reported in table 3 in Stumpp et al., 2012) was 250 days. Anyway, we cannot fully interpret the differences between the particle tracking algorithm and the virtual tracer experiment. In this study, we tried to understand the role of dispersivity in tracer transport simulations.

Using the original (actual) dispersivity allows the tracer transport simulation to be carried out under realistic conditions (Stumpp et al., 2012). The dispersivity is known to be a length-scale dependent parameter, and the impact of dispersivity on the advective-dispersive transit time still remains unclear. Therefore, we carried out a sensitivity analysis to estimate $\tau_R$, $\tau_D$, and $\tau_L$ by changing $\lambda_i$ (Figure 7). We found that RWU and evaporation transit times are weakly or poorly sensitive to dispersivity because water parcels are removed by evapotranspiration fluxes near the surface (roots are mostly distributed near the soil surface). By contrast, drainage transit time is positively correlated with dispersivity. In this case, water parcels travel across the entire depth of the soil profile and are highly influenced by dispersivity. The use of the original dispersivity in the virtual tracer experiment induced a faster downward movement of the tracer when compared to that of the particle (Figure 6a).

4.2 Future applications

In this study, we set up a modelling protocol to carry out a virtual tracer experiment which can be used to assess the temporal origin of RWU, evaporation, and drainage in plot-scale applications (Benettin et al., 2021). The results for each daily event can be aggregated at any desired temporal resolution to investigate the effects of climate seasonality on water balance and timing. We found that transpiration timing is driven by seasonal dynamics characterizing plant growth and dormancy. While it is well known that plants’ water supply is replenished by precipitation occurring in the dormant season under seasonal climate regimes, the temporal origin of water used by roots under temperate climates is still poorly understood (Brinkmann et al., 2018). Our results indicate that a key challenge in understanding hydrological processes in the critical zone is the determination of the water demographics (Sprenger et al., 2016). Indeed, a potential drought event in the growing season with a duration longer than the mean of the RWU transit time distribution could be detrimental to plant survival. Conversely, water falling during the dormant season could buffer the lack of precipitation in the growing season within the age distribution, which can range from a few days to several months (Brinkmann et al., 2018; Sprenger, Tetzlaff, Buttle, Laudon, Leistert, et al., 2018).

5 | CONCLUSIONS

The temporal origin of root water uptake, evaporation, and drainage water represents a functional indicator to quantify ecosystem vulnerability and resilience to changes in climate and land use. For instance, the impact of seasonal rainfall anomalies on the resilience of forest plantations is still uncertain. Plant reliance on past rainfall is important in season-dry climates and even in humid climates punctuated by drought. It is also essential to know how much rainwater percolates downward to the shallow aquifer and how much water is returned to the atmosphere through evapotranspiration to select the most cost-effective crops to save irrigation water during the growing season and simultaneously reduce groundwater pumping in cropland management. The main advantage of using virtual tracer experiments is the possibility of generating scenario modelling approaches that enable the impacts of natural and anthropogenic disturbances on the temporal origin of the water balance components to be assessed based on long-term (in the order of decades or centuries) simulations of water flow and tracer transport.

In this study, the temporal origin of water in the soil–plant–atmosphere continuum system was estimated using a synthetic approach based on tracer transport simulations carried out with a process-oriented hydrological model. Our three main findings reflect the three research questions and associated goals and may be summarized as follows:

- Drainage and RWU water transit times obtained using the virtual tracer experiment were compared to those obtained considering advection-dominated transport. On the one hand, the RWU transit times estimated by particle tracking and virtual tracer experiment agreed fairly well with relatively low errors. On the other hand, the assessment of drainage transit times using the two methods is still affected by large errors. The large errors are due to different model setups of the two approaches and tracer transport simulations being affected by dispersivity.
- The impact of dispersivity on tracer-based transit times was evaluated by conducting a sensitivity analysis. Such analysis must be considered, especially when dispersivities are unknown or assumed as 1/10th of the soil profile depth. While dispersivity strongly influences drainage transit times, its effect on evaporation and transpiration transit times is minimal. Large dispersivity values might exacerbate the differences between the particle tracking and virtual tracer experiment approaches. The actual dispersivity value...
calibrated in a previous study allows the implementation of the virtual tracer experiment, even though its value influences drainage transit times. We expect differences between the two methods to become larger when the investigated soil profile is deeper than 150 cm and the actual dispersivity is greater than 4.7 cm.

- The virtual tracer experiment integrates the RWU, evaporation, and drainage transit times with the corresponding rainfall partitioning for each rainfall event. This information needs to be assessed in soil profiles over space, interpolated, and mapped to get vulnerability and resilience indicators. The seasonal aggregation of the RWU temporal origin helped quantify two distinct frequency distributions, which can be used to assess the impact of climate variability on water storage dynamics in the critical zone.

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DATA AVAILABILITY STATEMENT

Data can be downloaded from the HYDRUS website (https://www.pc-progress.com/en/Default.aspx?h1d-lib-Isotope). Two open-source Matlab scripts are available. The PT.m Matlab code determines the drainage transit time based on the particle tracking algorithm, while the VTE.m Matlab code determines the drainage and RWU transit times and relative rainfall contributions to actual evaporation, actual transpiration, and drainage using isotope transport simulations in HYDRUS-1D (see details in Data S1).

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REFERENCES


SUPPORTING INFORMATION
Additional supporting information can be found online in the Supporting Information section at the end of this article.


APPENDIX A

<table>
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<th>TABLE A1</th>
<th>HYDRUS-1D input and output variables and files.</th>
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$P$ Particle positions in the soil profile