

Exploring source water mixing and transient residence time distributions of outflow and evapotranspiration with an integrated hydrologic model and Lagrangian particle tracking approach

Reed M. Maxwell¹  | Laura E. Condon²  | Mohammad Danesh-Yazdi³  | Lindsay A. Bearup⁴

¹ Colorado School of Mines, Golden, Colorado, USA

² University of Arizona, Tucson, Arizona, USA

³ Sharif University of Technology, Tehran, Iran

⁴ US Bureau of Reclamation, Denver Federal Center, Denver, Colorado, USA

Correspondence

Reed M. Maxwell, Colorado School of Mines, 1500 Illinois St, Golden, CO.
Email: rmaxwell@mines.edu

Funding information

Biological and Environmental Research, Grant/Award Number: DE-AC02-05CH11231; Sustainable Systems Scientific Focus Area; Offices of Advanced Scientific Computing Research and Biological and Environmental Sciences IDEAS project; U.S. Department of Energy Office of Science

Abstract

Understanding the time water takes as it moves from rain or snowmelt through the terrestrial system to arrive as stream discharge, or evapotranspiration (ET) is an important hydrologic quantity. We develop a Lagrangian particle tracking method to capture transient residence times from source to either ET or outflow in an integrated hydrologic model. This method is parallel and efficiently captures time evolution of parcels of water in the model and tracks the source of water for hydrograph or ET separation. We demonstrate this model using hypothetical hillslope simulations driven by snow or rain dominated forcing and two different land cover types. We show that land cover and forcing both impact the outflow residence time distribution, which spans many years. We also introduce the idea of ET residence time distributions and show that while mean ET residence times are typically less than 1 year, land cover affects this quantity and simulated ET processes draw from much older water (many years old) depending on location on the hillslope or seasonal cycle. Finally, we study source water contribution to outflow and ET and explore assumptions about a residence time-based definition of older, pre-event, or groundwater end member. We show that simulated plant processes may switch to more opportunistic and younger sources of water, changing the composition of outflow.

KEYWORDS

modelling, numerical, plant water use, residence time, source water contribution

1 | MOTIVATION

Untangling the mechanisms by which watersheds partition incoming precipitation to overland flow and evapotranspiration (ET) is a deceptively challenging open problem in hydrology. Better quantitative tools are needed to study the relationship between groundwater and stream chemistry, concentration discharge across flow regimes, and

groundwater subsidies to plant water use (Brooks et al., 2015). Observational evidence of isotopic differences in surface and plant water chemistry, as well as trade-offs between fast and slow flow processes highlight the complex multiscale behaviour of hydrologic systems. For example, recent observational work suggests that vegetation accesses sources of water under stress not previously considered (Bales et al., 2018; Bearup, Maxwell, Clow, & McCray, 2014; Fan, Miguez-Macho,

This is an open access article under the terms of the Creative Commons Attribution License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

© 2018 The Authors Ecohydrology Published by John Wiley & Sons Ltd

Jobbágy, Jackson, & Otero-Casal, 2017; Rempe & Dietrich, 2018). Water source has also been linked to differences in residence time within a watershed (e.g., Bearup, Maxwell, & McCray, 2016; Botter, Bertuzzo, & Rinaldo, 2010; Remondi, Kirchner, Burlando, & Fatichi, 2018); however, more work is needed to formally tie these concepts together and to observations. Improved prediction of watershed and ecosystem behaviour requires better prediction of the spatio-temporal dynamics of water availability.

To move forward, we need advances in both modelling and observations and novel approaches to identify functional differences and reconcile process understanding. Residence time distributions are well established tools that relate the time and travel paths water takes as it moves through the terrestrial system (Rinaldo et al., 2011). Techniques exist to solve these quantities analytically (e.g., Botter, Bertuzzo, & Rinaldo, 2011) and numerically (e.g., Cardenas, 2007; Kollet & Maxwell, 2008). Whereas much modelling work has focused on residence time distributions in steady state systems, travel time distributions in transient systems are much less explored (Engdahl, 2017; Engdahl, McCallum, & Massoudieh, 2016). Furthermore, most modelling studies focus on residence time distributions for stream discharge, very little work, to our knowledge, has studied the residence time distributions of ET or developed source water contributions to plant water use numerically.

Integrated hydrologic models can help unravel physical processes and interpret observations in complex nonstationary systems that cannot be solved analytically, and which can only be sparsely observed (Maxwell & Condon, 2016). In this way, we can use models to improve process understanding not just make predictions (Sivapalan, 2018). Here, we develop a new Lagrangian particle tracking approach that nests within an integrated hydrologic model. This model is designed to evaluate travel time distributions in transient model simulations. It computes flow paths and residence time distributions for time varying overland flow and evapotranspiration (ET) fluxes. In addition to computing residence times, the model also tracks the source water (i.e., rain, snow, and groundwater) for every outflow. This model is fully transient and can be driven by observed meteorological forcing. We present this numerical approach and demonstrate it using idealized hillslope simulations.

2 | METHODS: MODEL DESCRIPTION

The new model presented here, EcoSLIM,¹ is a transient Lagrangian particle tracking model designed to nest within an integrated hydrology model, in this case ParFlow-CLM. The overall approach is similar to the steady-state approach described in Danesh-Yazdi (Danesh-Yazdi, Klaus, Condon, & Maxwell, 2018) and the transient approach developed in Bearup et al. (2016). EcoSLIM uses spatially gridded pressure, saturation, subsurface flow velocity, precipitation and evapotranspiration fluxes, and land surface states output from the integrated hydrologic model at every timestep to insert, move, and remove particles from the domain. EcoSLIM tracks particles through each control volume in the domain with an optimal local timestep used for each particle based on a prior version of the code SLIM (Kollet & Maxwell, 2008; Maxwell & Kastenbergh, 1999; Maxwell, Welty, &

Harvey, 2007). Here, the previous SLIM model is reformulated to (Bales et al., 2018) handle transient velocity fields in the subsurface, (Bearup et al., 2014) dynamically insert particles into the domain with precipitation events, and (Bearup et al., 2016) track source water contributions in addition to residence times.

The methodology presented here is general and could be written in any language, but we chose modern Fortran with Open-MP² thread parallelism for portability, high performance, and good parallel scaling (see Appendix A). The model is released free and open source using the GNU Lesser General Public License v3.0. Similarly, EcoSLIM is a generic particle tracking code that could use outputs from any integrated hydrology model with land surface processes, but for illustrative purposes, we demonstrate using the ParFlow platform.³ ParFlow is an integrated groundwater surface water model, and here, we apply ParFlow configured with the CLM land surface model. The coupled ParFlow-CLM model simulates hydrologic processes from the bedrock to the top of the canopy. Particles are added or removed at every ParFlow-CLM timestep depending on the fluxes that occur across the land surface boundary (i.e., canopy throughfall or direct precipitation infiltrating to subsurface, evapotranspiration transmitting water from the subsurface to the atmosphere and overland flow).

Particles are added to the domain in one of two ways providing variety in experimental design. First, the user specifies the number of particles to initialize within each subsurface grid cell, and particles are assigned a random location within the cell and are tagged as “groundwater.” This results in a particle mass related to the quantity of water represented by a given particle, $m_p = \frac{1}{n_i} \Delta x \Delta y \Delta z \rho \theta S_s$ [M], where Δx , Δy , and Δz are the cell dimensions [L], ρ is the density of water [ML⁻³], θ is the effective porosity [-], S_s the saturation of water in that cell [-], and n_i is the number of particles added [-]. Second, particles are added throughout the transient simulation when and wherever there are positive fluxes into the subsurface (indicating recharge from a precipitation event) resulting in $m_p = \frac{Q_i}{n_i} \Delta x \Delta y \Delta z \rho \theta S_s$ where Q_i is the flux of new water [T⁻¹] over a timestep Δt [T]. In this case, the user specifies the number of particles, n_i , to be added per grid cell when positive fluxes occur with better particle resolution occurring with larger values of n_i . Although n_i is a user-adjustable parameter, large values result in better resolution of water inputs but longer simulation times. These particles are tagged as either rain or snow depending on precipitation type in ParFlow-CLM. All particles are initialized with a randomly assigned age (between zero and Δt) at the time they are added. Particle masses are variable and scale with the input fluxes. This approach ensures appropriate mass weighting in residence time and source water distributions. Particles initialized in the subsurface are given a mass equivalent to the initial water storage in the cell divided by the number of initialized particles. Particles added for transient recharge events are assigned a mass equivalent to the flux of water into a grid cell multiplied by the density of water when added to the domain. Assigning m_p using the flux of water that enters at each cell is consistent with a flux-weighted approach often used in streamlines with traditional particle tracking based on mass.

¹<https://github.com/reedmaxwell/EcoSLIM>

²<https://www.openmp.org/about/openmp-faq/>

³<https://parflow.org>

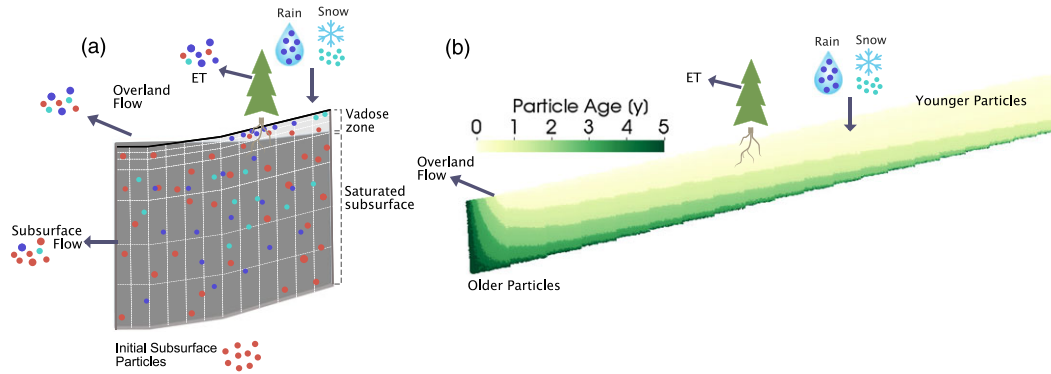


FIGURE 1 (a) Schematic of particle tracking method and (b) example of particle age distribution during a simulation

Once added to the domain, particles move through advection, dispersion, and diffusion driven by the transient ParFlow-CLM velocities. Particles move via the Ito–Fokker–Planck approximation to the advection–dispersion equation in a manner detailed previously (see, e.g., supporting information in Maxwell et al., 2007) and summarized briefly here. Generally

$$X_p(t + \Delta t) - X_p(t) = \left[\mathbf{v}_p + \nabla \cdot \mathbf{D} + \frac{\mathbf{D}}{\theta S_s} \cdot \nabla \theta S_s \right] \Delta t + \mathbf{B} \cdot \mathbf{z} \sqrt{\Delta t}, \quad (1)$$

where $X_p(t)$ [L] is the location of each particle at time t [T]; $\mathbf{v}_p$ is the local velocity [LT^{-1}] at the particle location; $\mathbf{D}$ is the dispersion tensor approximated by $\mathbf{D} \approx (\alpha_L \mathbf{v} + D_e) \mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{v} \mathbf{v}}{v}$ where α_L and α_T are the longitudinal and transverse dispersivities [L], v is the magnitude of the velocity [LT^{-1}], D_e is an effective molecular diffusivity [$\text{L}^2 \text{T}^{-1}$], $\mathbf{B}$ is defined as $\mathbf{B} \cdot \mathbf{B}^T = 2\mathbf{D}$, and $\mathbf{z}$ is a random vector with zero mean and unit variance. If dispersion and diffusion terms are neglected, we arrive at Equation (4) in Danesh-Yazdi et al. (2018). For the examples shown, we neglect macrodispersion but include effective molecular diffusion, arriving at

$$X_p(t + \Delta t) - X_p(t) = \mathbf{v}_p \Delta t + \mathbf{z} \sqrt{D_e 2 \Delta t} \quad (2)$$

Each particle is moved independently using first order advection, linearly interpolating the cell-interface velocities to the exact particle location (Danesh-Yazdi et al., 2018). Individual particle timesteps (Δt in 2) are chosen based on a maximum local stability criterion that is different for every movement. All active particles are regrouped at set intervals (a macro timestep) either when output is needed or the velocity forcing changes. Particle movements are conducted in parallel using Open-MP in thread-safe loops. The age of each particle increases linearly as long as the particles are active. All particle states (e.g., age, source, and mass) are aggregated to arrays based on the ParFlow-CLM computational grid to be written at defined intervals, along with complete domain statistics (mean age, all changes in particle states) written at every ParFlow-CLM timestep. Individual particle locations may also be written at defined intervals, up to every forcing timestep.

A particle becomes inactive when it leaves the domain, either by (Bales et al., 2018) outflow from the subsurface, (Bearup et al., 2014) overland flow, or (Bearup et al., 2016) ET. Fluxes that point out of

the domain in the subsurface are characterized as outflow, otherwise particles are reflected at boundaries. Particles that reach a ponded cell (i.e., a surface cell with overland flow) are characterized as overland flow and removed from the simulation. Negative fluxes in ParFlow-CLM indicate removal of water by ET. These fluxes are handled like a partially penetrating well in traditional groundwater simulations where $= \frac{Q_{et} \Delta t}{\Delta x \Delta y \Delta z \rho \theta S_s}$. Here, the volumetric ET flux Q_{et} [$\text{L}^3 \text{T}^{-1}$] is compared with the quantity of water in each cell normalized by the time step length for each particle within the cell. A random number, $\mathbf{z}$, is generated, and if this number is greater than this normalized quantity, $P_{capture}$, the particle is removed via ET. The mass of the particle, m_p , is multiplied by its corresponding age and source to generate an ET flux breakthrough. If a sufficient number of particles are used, the mass of particles leaving the domain as outflow and ET should equal the outflow and ET flux from the integrated hydrologic simulation. Particles are sorted every timestep recycling those that have exited to allow the total array size to be stable throughout the simulation. With this approach, a particle distribution is generated for every flux out of the model (subsurface flow, overland flow, and ET) for every time step and spatial location. This allows for the calculation of dynamic mass weighted residence time distributions that vary spatially and the explicit tracking within distributions of source water contribution.

3 | METHODS: SIMULATION APPROACH

To demonstrate the EcoSLIM code, we run four synthetic hillslope cases. The hillslopes are not intended to mimic an actual site. They are designed to illustrate the spatio-temporal behaviour of outflow and ET residence time distributions, and source water contribution that can be captured with this approach. The four demonstration hillslopes all have the same geometry: 100 m in x , 1 m in y , and 9.4 m in z with a constant slope of 0.1 in the x -direction (Figure 1). Discretization is $n_x = 20$, $n_y = 5$, and $n_z = 20$ with constant $\Delta x = 5$ m, $\Delta y = 0.2$ m, and a variable Δz that is 0.5 m for the bottom 9 m of the domain (i.e., 18 layers) and 0.3 and 0.1 m for the top two layers moving up. All simulations were populated with homogeneous parameters, saturated hydraulic conductivity $K_{sat} = 0.05$ [mh^{-1}], Manning's $N = 10^{-6}$ [$\text{m}^{1/3} \text{h}^{-1}$], porosity $\theta = 0.2$ [–], and van Genuchten parameters $\alpha = 1.0$ [m^{-1}] and exponent $n = 2.0$ [–]. Boundary conditions for ParFlow and EcoSLIM were no-flow on the bottom and sides, allowing

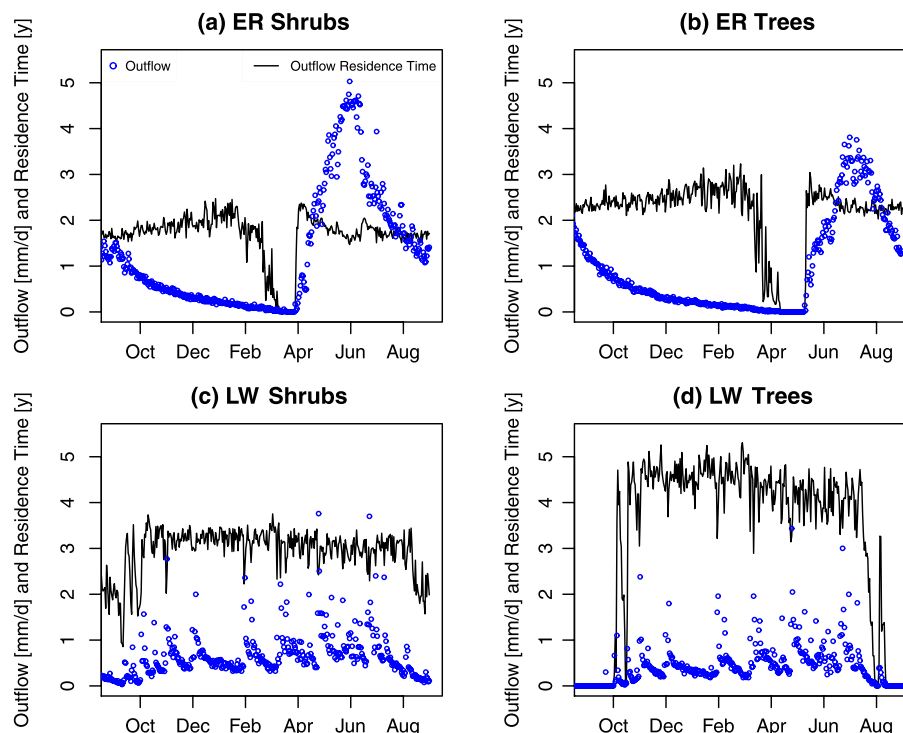


FIGURE 2 Plot of daily mean outflow residence time and outflow for the (a) *ER Shrubs*, (b) *ER Trees*, (c) *LW Shrubs*, and (d) *LW Trees* cases

water to exit only via ET or surface outflow. This hillslope simulation approach is generally very similar to prior studies (Bearup et al., 2016; Pribulick et al., 2016). EcoSLIM was configured to place two particles per cell per precipitation event and a maximum of 3M particles (though this maximum was never reached). The local timesteps for each particle move were limited to a maximum of $\Delta x_{y,z}/v_{x,y,z} = 0.25$ [T].

Two real meteorological forcing datasets were used to drive ParFlow-CLM: one for a high elevation, snow-dominated mountain headwaters (East River, Colorado), *ER*, (Pribulick et al., 2016) and one for a semiarid, rain-dominated plains system (Little Washita, Oklahoma), *LW*, (Condon & Maxwell, 2014). Two homogeneous land-cover types were specified, one with the Evergreen Needleleaf plant functional type (*Trees*) and one with the Shrub plant functional time (*Shrubs*). These land cover types were chosen more for their differences in rooting depth distribution than for their applicability to the actual vegetation present at either forcing dataset location. Details on the root zone distribution and uptake within ParFlow-CLM using the rescaled model formulation are given in Ferguson, Jefferson, Maxwell, & Kollet (2016). ParFlow-CLM⁴ was used to simulate all flow processes and was run for 5 consecutive years repeating a single year of hourly forcing. At the end of the period, all four cases had reached a dynamic equilibrium, and the water balance over the water year was closed within 1% of precipitation.

Because EcoSLIM operates independently from ParFlow-CLM, any sequence of the outputs from the hydrologic simulation can be repeated as many times as desired within the EcoSLIM particle simulation. In this experiment, the final year of hourly ParFlow-CLM simulation output was used to repeatedly drive EcoSLIM for 20 years (see

Appendix B for details). At the end of the 20-year particle simulation, the mean particle ages for each case were no longer changing, and the EcoSLIM system was determined to be fully spun up. Only this final year of EcoSLIM simulation is presented in the results. The number of particles was allowed to grow to steady state as dictated by the conditions of each simulation (i.e., the number of precipitation events and balance of inflow and outflow). All simulations had between one and two million active particles at steady state. All simulations were run on a MacPro desktop; ParFlow simulations took approximately 1 hr of wall-clock time to complete 5 years of simulation time (with hourly forcing), whereas EcoSLIM simulations took approximately 3.5 hr of wall-clock time to run a 20-year simulation. All simulations were run on one processor, but EcoSLIM was allowed to run up to eight threads on that processor.

4 | RESULTS AND DISCUSSION

Here, we present results from the four test cases that cover two climate types (*ER* and *LW*) and two land cover types (*Trees* and *Shrubs*). Results illustrate the functional behaviour of EcoSLIM and highlight the utility of this tool for quantifying spatial and temporal hillslope behaviour. Comparisons between test cases highlight interactions between vegetation and climate that create systematic differences in hydrologic behaviour.

Figure 2 plots the mean residence time for all particles that leave the domain as outflow for each simulation day and all four cases. The full distribution of these particle residence times is discussed in detail later. We see that the mean outflow residence time distributions display several scales of temporal variability. The *ER* cases (Panels A and B) show a clear seasonal cycle with peak flows occurring in the spring, consistent with a snowmelt dominated basin. The *LW* cases

⁴<https://github.com/parflow/parflow>

(Panels C and D) show less of a seasonal cycle but exhibit clear fluctuations in mean outflow residence time following individual precipitation events consistent with a rainfall dominated system. We see that the *ER* forcing results in a smaller mean outflow residence time than the *LW* forcing (comparing, e.g., Panels A and C). This is likely due to differences in overall aridity between the two forcings (the difference between precipitation and evapotranspiration [P-ET] for *LW* cases is smaller than for the *ER* cases) similar to the steady-state behaviour shown previously (see Figure 6 in Danesh-Yazdi et al., 2018). We also see a distinct impact of vegetation with *Trees* cases having larger mean outflow residence times than *Shrubs* cases (comparing, e.g., Panels C and D). This behaviour is likely due to the larger ET and smaller throughfall exhibited by the *Trees* cases for both forcings, making overall P-ET smaller.

Figure 3 depicts the mean daily residence time for all particles that leave the domain as ET for each simulation day and all four cases. The full distribution of ET residence times varies both spatially and temporally, as discussed below. We see that mean ET residence time is smaller (younger) and exhibits more temporal variability than mean outflow residence time (comparing Figures 2 and 3). The mean ET residence times are typically less than 1 year except for the *Trees* land cover cases (Panels B and D) indicating that on average, simulated plants with deeper root structures are able to access older water. The *ER* forcing cases show a very clear seasonal cycle in mean ET residence time with the oldest water being used for ET just prior to snowmelt. During snowmelt, mean residence times decrease sharply (May, Panels A and B) indicating simulated ET is composed of recent meltwater (this will also be explored later). The *LW* forcing shows a different seasonal cycle than *ER* due to being primarily rain fed with rapid fluctuations in residence time (Jun to August, Panels C and D).

Figure 4 plots monthly residence time distributions over the water year for *ER* and *LW* forcing for the *Trees* land cover type. In contrast to Figures 2 and 3, which only plot the mean of the outflow and ET residence times, Figure 4 represents monthly snapshots of the full distribution of outflow residence times (Panels A and C) and ET (Panels B and D). This figure shows a long tail for outflow and ET indicating that all four residence time distributions contain some fraction of older water. We also see systematic shifts in residence time distribution over the course of the year that depend on the atmospheric forcing. The *ER* outflow forcing case shows several distinct peaks driven for every month except May during which snowmelt appears to mix residence times (Figure 4a). For the *ER* forcing, the multiple peaks in Figure 4 demonstrate that the outflow residence distribution contains information about several prior years of forcing. This concept is emphasized in this simulation because the *ER* forcing is snowmelt dominated and the same water year of forcing is repeated for 20 years creating a somewhat artificial but illustrative residence time distribution. The *LW* outflow residence time distributions (Figure 4c) also show influence from prior forcing but the peaks are less distinct and the seasonal changes in outflow residence time less pronounced. The *ER* ET residence time distributions demonstrate a clear seasonal cycle (Figure 4b) where mean residence times increase until May at which point ET residence time distributions show multiple peaks. The *LW* residence time distributions (Figure 4d) do not demonstrate a clear seasonal cycle but do contain small fractions of older (up to 10 years) water throughout.

To further explore the small fraction of older (>2 years) water present in all ET distributions, Figure 5 plots the distribution of ages spatially for all four cases. This figure shows that the distribution of ages up the hillslope (the y-axis in this figure) exhibit a clear pattern.

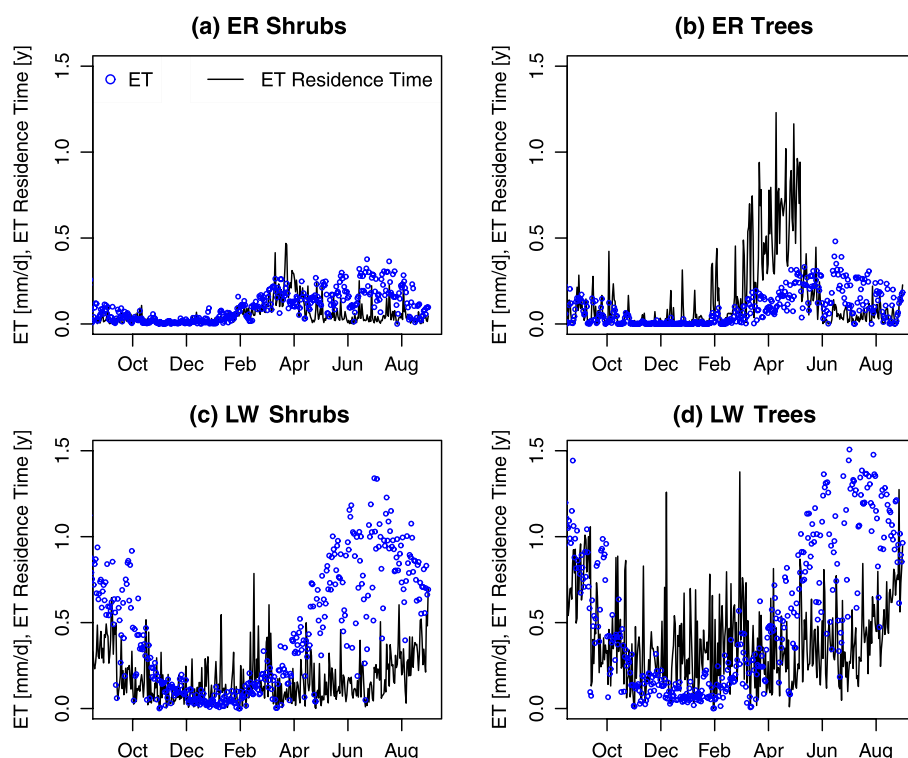


FIGURE 3 Plot of daily, domain averaged ET residence time and ET for the (a) *ER Shrubs*, (b) *ER Trees*, (c) *LW Shrubs*, and (d) *LW Trees* cases

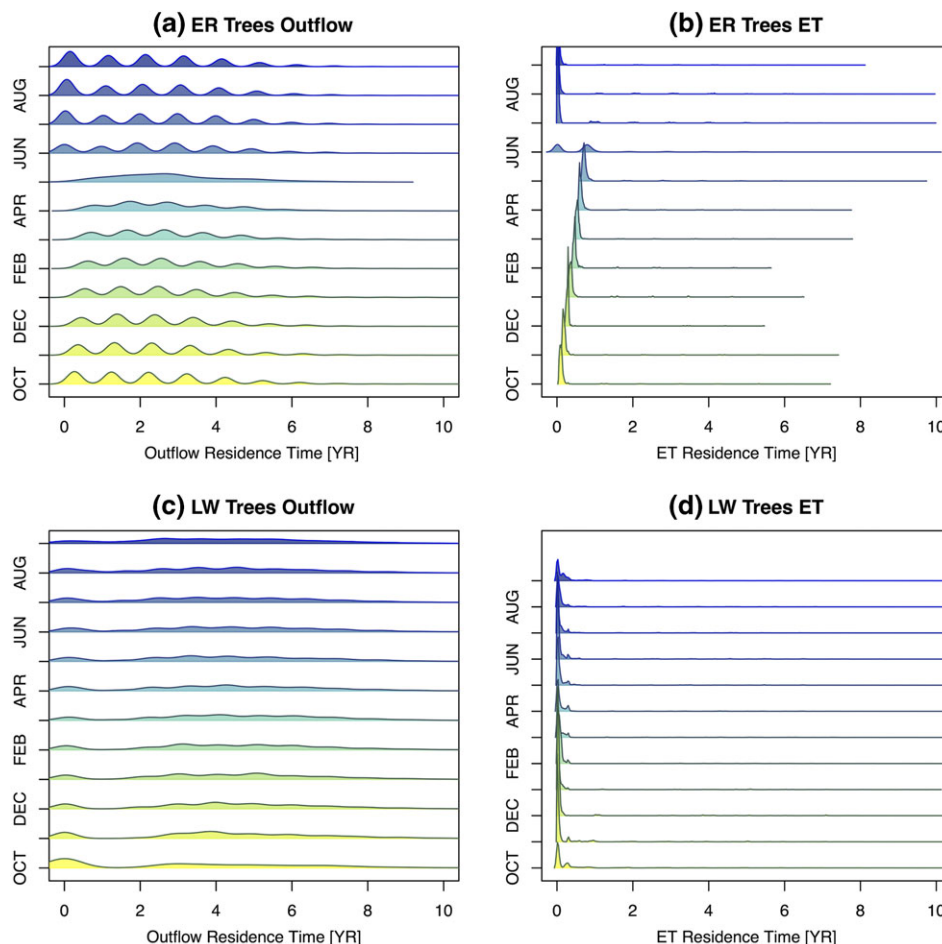


FIGURE 4 Plot of monthly distributions of residence time for the (a) ER outflow, (b) ER ET, (c) LW outflow, and (d) LW ET cases. Note all cases are for the *Trees* land cover type

In all cases, simulated ET from vegetation in the upper portions of the hillslope draws from younger water while plants on the lower portion of the hillslope accesses water that is multiple years old. Within this general trend, spatial patterns of ET residence time distribution also vary with forcing and with vegetation type. The *ER* forcing cases (Figure 5a,b) show distinct peaks that correspond with each water year, whereas the *LW* forcing (Figure 5c,d) is more mixed. Vegetation with deeper root zone distributions (*Trees* cases, Figure 5b,d) use older water for ET at locations farther up the hillslope than shallower root zone systems (*Shrubs* cases, Figure 5c,d). For example, the *LW Trees* case (Figure 5d) shows ET residence times of approximately 2 years old at a location of $x = 40$ m, while the ET in the *LW Shrubs* case (Figure 5c) is composed of younger water.

Figure 6 plots outflow and ET for the *ER Shrubs* case in a stacked plot by the particle source (rain, snow, or groundwater) for Year 20 of the simulation. We explore two different classifications for which particles represent groundwater or old water. Initially, all particles are tagged as either “groundwater” (i.e., particles initialized in the subsurface at the start of the simulation), rain, or snow (depending on how a particle gets added). Here, we reclassify rain and snow particles as groundwater after they have spent a set amount of time in the subsurface. Figure 6 illustrates the application of two different thresholds: (a) reclassifying all particles greater than 1 year as groundwater (the young groundwater Cases A and B in Figures 6 and 2) reclassifying

all particles greater than 5 years as groundwater (the old groundwater Cases C and D in Figure 6). An alternate way to conceptualize this approach is that we assume source water retains its original signature (i.e., rain or snow) for some amount of time before this is erased and it becomes older water (i.e., groundwater), mimicking what might happen if the water attributes carry some signature that decays with time or increases with contact time to some subsurface material. The choices of 1 and 5 years are completely arbitrary and used for illustrative purposes. Figure 6a,b shows sources of water contributions to outflow and ET for the two classification systems. We see that groundwater (water greater than 1 year old) makes up the majority of outflow (Figure 6a,b), with snowmelt (less than a year old) making up the next largest fraction and rainfall (less than a year old) making up a very small portion of outflow water. Figure 6a shows that simulated outflow contributions vary substantially over the water year, with snowmelt contributions peaking during snowmelt and decreasing during the summer and baseflow. Figure 6b shows that ET is comprised mostly of snowmelt water (less than 1 year old) but with a significant fraction of water that is greater than 1 year old. Figure 6c,d shows the numerical hydrograph separation for old groundwater (greater than 5 years). These figures show that the old water portion of the outflow hydrograph is small, though still present and that very little water used by ET is greater than 5 years old. For this assumption, both outflow and ET are primarily composed of water that originated

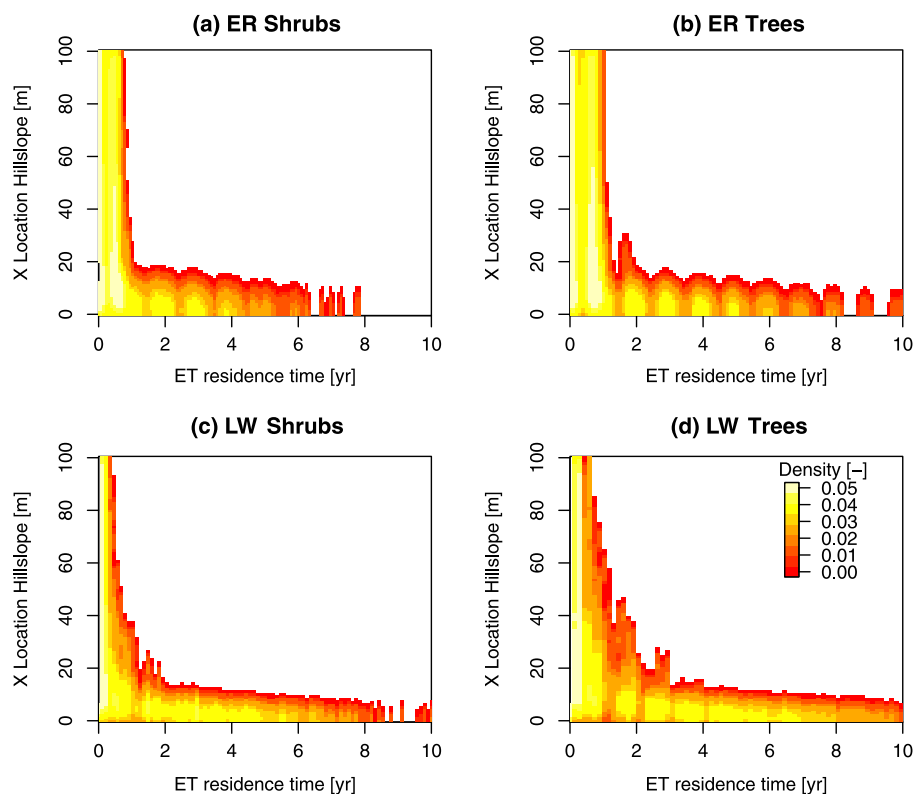


FIGURE 5 Probability Density Function (PDF) of ET residence time along the hillslope for the (a) *ER Shrubs*, (b) *ER Trees*, (c) *LW Shrubs*, and (d) *LW Trees* cases. Note in this figure, the y-axis is the spatial location along the hillslope, the x-axis is ET residence time, and the colours are probability density with yellow being greater probability, red lesser, and white zero

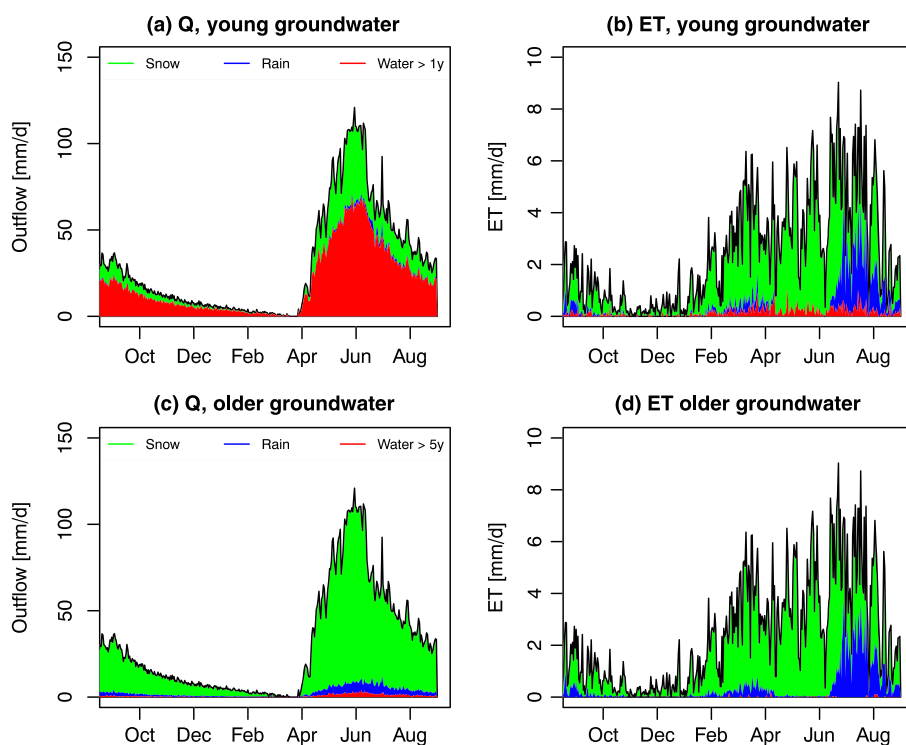


FIGURE 6 Plots of source water contribution for outflow (a,c) and ET (b,d) for the *ER Shrubs* case with source attribution by snow (green), rain (blue), and pre-event groundwater or older water (red). Note that Cases A and B assume that pre-event water is older than a year, while Cases C and D retain the original source water for up to 5 years

as snow. A large portion of water that originated as rain is used for mid to late summer ET (Figure 6b,d) suggesting that simulated ET draws preferentially from younger water if it is available. These rain parcels of water are taken up by ET first in the model and therefore do not flow to the outlet. This finding illustrates how plants simulated in the model draw from more easily available water sources preferentially, even when plant water use is dictated by the hydrology in the relatively simple manner used here.

5 | CONCLUSIONS AND NEXT STEPS

Here, we present a Lagrangian model that tracks water through an integrated hydrologic simulation. This new code, EcoSLIM, expands on previous tools to provide insight into transient outflow and ET residence time distributions and source water contributions. Simple, hypothetical hillslope simulations with variations in land cover and atmospheric forcing were used to explore the system behaviour and illustrate the complexity that can be captured with this approach. Although the homogenous simulations used here are intentionally idealized, some interesting insights can still be drawn from this study:

- Water that left the hillslope domain was composed of a range of age in all cases with ET mean residence times being shorter than outflow residence times.
- For our experiments, the *LW* rain-fed cases produced older residence times than the *ER* snowmelt cases; changes in atmospheric forcing had less of an impact on ET residence time than on outflow residence time distributions.
- The land cover type cases with deeper root systems (*Trees*) resulted in older ET residence time distributions than the shallower root distribution cases (*Shrubs*); changes in land cover changed outflow residence time distributions.
- The distribution of residence times for outflow evolved seasonally.
- Source water partitioning is very sensitive to the assumed age of groundwater.
- ET from locations at the bottom of the hillslope sourced much older water than at the top of the hillslope.
- Plants simulated in the model drew from more easily available water sources preferentially.

Findings from the simple test cases here illustrate the potential for this approach to be applied to larger watershed simulations. Moving forward, it is important to use this platform to simulate real domains and to compare to observations (e.g., Benettin, Kirchner, Rinaldo, & Botter, 2015; Böhlke & Denver, 1995; Carroll et al., 2018; Remondi et al., 2018). Validation of any modelling exercise is important and datasets to compare high frequency observations of outflow water age to a model such as EcoSLIM are still growing in number. An even larger challenge is to observe the age of ET, and to our knowledge, no comprehensive study of ET residence yet exists. This provides an opportunity for model prediction to perhaps guide these observations. As EcoSLIM is written efficiently and in parallel, we have already

tested it for very large domains with ~100M particles and hundreds of compute cores. The relationships illustrated here, such as the change in residence time distribution with land cover or spatial differences in ET residence time are testable and would provide a window into the physical assumptions applied in physical hydrology models. Additional studies focused around topographic, land cover and subsurface heterogeneity would elucidate these controlling factors. We see many opportunities to apply EcoSLIM to hydrologic simulations and better bridge outflow and ET residence time simulation and ecohydrological process.

ACKNOWLEDGEMENTS

All codes and model output are publicly available on GitHub.⁵ The inputs for the four hillslope cases used are part of the EcoSLIM repository along with R scripts to read output and create basic plots. This work was supported by the U.S. Department of Energy Office of Science, Offices of Advanced Scientific Computing Research and Biological and Environmental Sciences IDEAS project, and the Sustainable Systems Scientific Focus Area under Award Number DE-AC02-05CH11231.

ORCID

Reed M. Maxwell  <http://orcid.org/0000-0002-1364-4441>

Laura E. Condon  <http://orcid.org/0000-0003-3639-8076>

Mohammad Danesh-Yazdi  <http://orcid.org/0000-0003-2918-7713>

REFERENCES

- Bales, R. C., Goulden, M. L., Hunsaker, C. T., Conklin, M. H., Hartsough, P. C., O'Geen, A. T., ... Safeeq, M. (2018). Mechanisms controlling the impact of multi-year drought on mountain hydrology. *Scientific Reports*, 8(1), 690.
- Bearup, L. A., Maxwell, R. M., Clow, D. W., & McCray, J. E. (2014). Hydrological effects of forest transpiration loss in bark beetle-impacted watersheds. *Nature Climate Change*, 4(6), 481–486.
- Bearup, L. A., Maxwell, R. M., & McCray, J. E. (2016). Hillslope response to insect-induced land-cover change: An integrated model of end-member mixing. *Ecohydrology*, 9(2), 195–203.
- Benettin, P., Kirchner James, W., Rinaldo, A., & Botter, G. (2015). Modeling chloride transport using travel time distributions at Plynlimon, Wales. *Water Resources Research*, 51(5), 3259–3276.
- Böhlke, J. K., & Denver, J. M. (1995). Combined use of groundwater dating, chemical, and isotopic analyses to resolve the history and fate of nitrate contamination in two agricultural watersheds, Atlantic Coastal Plain, Maryland. *Water Resources Research*, 31(9), 2319–2339.
- Botter, G., Bertuzzo, E., & Rinaldo, A. (2010). Transport in the hydrologic response: Travel time distributions, soil moisture dynamics, and the old water paradox. *Water Resources Research*, 46(3), W03514.
- Botter, G., Bertuzzo, E., & Rinaldo, A. (2011). Catchment residence and travel time distributions: The master equation. *Geophysical Research Letters*, 38(11). <https://doi.org/10.1029/2011GL047666>
- Brooks, P. D., Chorover, J., Fan, Y., Godsey, S. E., Maxwell, R. M., McNamara, J. P., & Tague, C. (2015). Hydrological partitioning in the critical zone: Recent advances and opportunities for developing transferable understanding of water cycle dynamics. *Water Resources Research*, 51(9), 6973–6987.
- Cardenas, M. B. (2007). Potential contribution of topography-driven regional groundwater flow to fractal stream chemistry: Residence time distribution analysis of Toth flow. *Geophysical Research Letters*, 34(L0540).

⁵<https://github.com/reedmaxwell/EcoSLIM>

- Carroll, R. W. H., Bearup, L. A., Brown, W., Dong, W., Bill, M., & Williams, K. H. (2018). Factors controlling seasonal groundwater and solute flux from snow-dominated basins. *Hydrological Processes*, 32, 2187–2202.
- Condon, L. E., & Maxwell, R. M. (2014). Feedbacks between managed irrigation and water availability: Diagnosing temporal and spatial patterns using an integrated hydrologic model. *Water Resources Research*, 50(3), 2600–2616.
- Danesh-Yazdi, M., Klaus, J., Condon, L. E., & Maxwell, R. M. (2018). Bridging the gap between numerical solutions of travel time distributions and analytical storage selection functions. *Hydrological Processes*, 32(8), 1063–1076.
- Engdahl, N. B. (2017). Transient effects on confined groundwater age distributions: Considering the necessity of time-dependent simulations. *Water Resources Research*, 53(8), 7332–7348.
- Engdahl, N. B., McCallum, J. L., & Massoudieh, A. (2016). Transient age distributions in subsurface hydrologic systems. *Journal of Hydrology*, 543, 88–100.
- Fan, Y., Miguez-Macho, G., Jobbágy, E. G., Jackson, R. B., & Otero-Casal, C. (2017). Hydrologic regulation of plant rooting depth. *Proceedings of the National Academy of Sciences*, 114(40), 10572–10577.
- Ferguson, I. M., Jefferson, J. L., Maxwell, R. M., & Kollet, S. J. (2016). Effects of root water uptake formulation on simulated water and energy budgets at local and basin scales. *Environmental Earth Sciences*, 75(4), 1–15.
- Kollet, S. J., & Maxwell, R. M. (2008). Demonstrating fractal scaling of baseflow residence time distributions using a fully-coupled groundwater and land surface model. *Geophysical Research Letters*, 35(7), 6.
- Maxwell, R. M., & Condon, L. E. (2016). Connections between groundwater flow and transpiration partitioning. *Science*, 353(6297), 377–380.
- Maxwell, R. M., & Kastenber, W. E. (1999). Stochastic environmental risk analysis: An integrated methodology for predicting cancer risk from contaminated groundwater. *Stochastic Environmental Research and Risk Assessment*, 13(1–2), 27–47.
- Maxwell, R. M., Welty, C., & Harvey, R. W. (2007). Revisiting the cape cod bacteria injection experiment using a stochastic modeling approach. *Environmental Science & Technology*, 41(15), 5548–5558.
- Pribulick, C. E., Foster, L. M., Bearup, L. A., Navarre-Sitchler, A. K., Williams, K. H., Carroll, R. W. H., & Maxwell, R. M. (2016). Contrasting the hydrologic response due to land cover and climate change in a mountain headwaters system. *Ecohydrology*, 9(8), 1431–1438.
- Remondi, F., Kirchner, J. W., Burlando, P., & Fatichi, S. (2018). Water flux tracking with a distributed hydrological model to quantify controls on the spatiotemporal variability of transit time distributions. *Water Resources Research*, 54(4), 3081–3099.
- Rempe, D. M., & Dietrich, W. E. (2018). Direct observations of rock moisture, a hidden component of the hydrologic cycle. *Proceedings of the National Academy of Sciences*, 115, 2664–2669.
- Rinaldo, A., Beven, K. J., Bertuzzo, E., Nicotina, L., Davies, J., Fiori, A., ... Botter, G. (2011). Catchment travel time distributions and water flow in soils. *Water Resources Research*, 47(7).
- Sivapalan, M. (2018). From engineering hydrology to Earth system science: Milestones in the transformation of hydrologic science. *Hydrology and Earth System Sciences*, 22(3), 1665–1693.

How to cite this article: Maxwell RM, Condon LE, Danesh-Yazdi M, Bearup LA. Exploring source water mixing and transient residence time distributions of outflow and evapotranspiration with an integrated hydrologic model and Lagrangian particle tracking approach. *Ecohydrology*. 2019;12:e2042. <https://doi.org/10.1002/eco.2042>

APPENDIX A

ECOSLIM PARALLEL SCALING

To assess parallel scaling, an experiment was conducted using a real domain with 2.7M particles. This test case was run in serial (one thread) and in parallel out to 32 threads. While this is a modest parallel scaling study, it illustrates the parallel efficiency of EcoSLIM. Figure A1

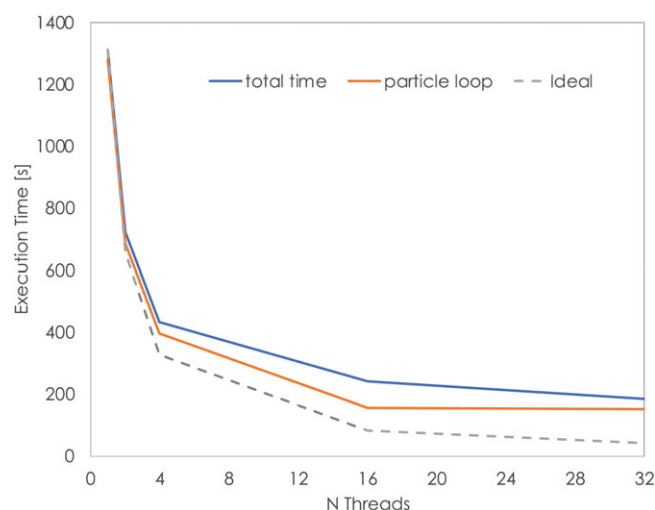


FIGURE A1 EcoSLIM exhibits good parallel speedup for a modest threadcount. Plot of total execution time, the execution time for just the parallel particle loop and an ideal speedup curve for 1 to 32 threads

plots the execution time for both the entire code and just the parallel section (which excludes initialization, and reading and writing files) along with the ideal speedup curve. We see good parallel scaling out to 16 threads, after which the scaling curve plateaus. This diminishment in speedup could be due to a number of factors including processor oversubscription and the small number of particles (2.7M) used in the experiment.

APPENDIX B

INITIAL PARTICLE AGE DISTRIBUTION AND ECOSLIM SPINUP PROCESS

Characterizing the distribution of water age within a catchment is challenging. For the simulations presented here, the distribution of

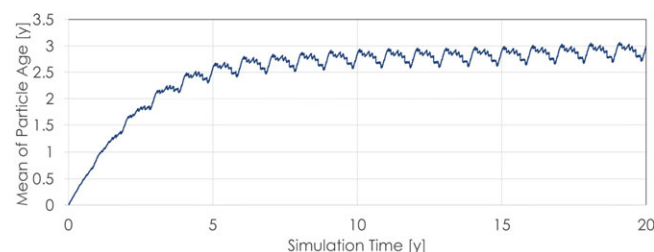


FIGURE B1 Plot of the 20-year EcoSLIM spinup for the LW Trees case. The mean age of all particles in the simulation is plotted as a function of simulation time

particle ages was spun up. The final year of the ParFlow-CLM hourly flow output was repeated for 20 years driving EcoSLIM. Particles were initialized everywhere and given an initial age of zero. Particles are added via precipitation and removed via ET or outflow until the mean age of the particles stabilized. As shown in Figure B1 for the *LW Trees* case, the mean particle age grows linearly for about the first five

simulation years with little impact from seasonality on the mean age. The annual change in mean age becomes smaller than the seasonality, and converges at which point we considered the simulation spun up; Figure 1b provides an example of the spatial distribution of these particle ages.