RESEARCH ARTICLE

Key Points:

- Accurate estimation of vegetation parameters is critical for simulation of the hydrologic cycle in land surface models
- Xylem water isotopic observations are used to calibrate plant hydraulic parameters for a forested stand of Eastern hemlock
- Integrated model-field research can guide field sampling strategies to obtain the most representative xylem isotopic data

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Parameterizing Vegetation Traits With a Process-Based Ecohydrological Model and Xylem Water Isotopic Observations

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Abstract Knowledge of plant hydraulic traits is critical for simulating terrestrial water storage, ecosystem water use, and tree responses to drought. The isotopic composition of tree xylem water (δ_{XYLEM}) has proven to be useful for understanding rooting strategies and for tracing terrestrial water flowpaths. Despite the broad collection of δ_{XYLEM} observations, few studies have estimated other plant traits from these data. We demonstrate the sensitivity of process-based isotope-enabled ecohydrological model (EcH$_2$O-iso) simulations of rooting depth distributions (K_{ROOT}), maximum stomatal conductance (gs_{MAX}), optimal growth temperatures (T_{OPT}), canopy light interception (K_{BEERS}), stomatal sensitivity to vapor pressure deficits (gs-VPD), and tree water storage capacity ($TreeV$) to δ_{XYLEM} observations. We sampled the δ_{XYLEM} of 30 Eastern hemlock (*Tsuga canadensis*) trees across 7 months, spanning a range of topographic positions and diameters. We calibrated the model 30 times with δ_{XYLEM} from each sampled tree. Calibrated values for gs_{MAX}, K_{BEERS}, and K_{ROOT} were validated with independent datasets of latent heat flux, canopy light interception, and xylem observations from independent hemlock stands. The calibrated values of several vegetation traits were significantly correlated with the diameters and topographic positions of the trees sampled in the field. These results indicate that δ_{XYLEM} reflects the characteristics and locations of the individual trees that are sampled, and therefore care must be taken in upscaling calibrated or measured plant traits for individual trees to larger horizontal scales. This research demonstrates that isotope-enabled hydrological-, land surface-, and Earth systems-models can leverage widely available water isotopic data to accurately estimate plant hydraulic traits.

Plain Language Summary Plants exert significant control over the amount of water stored in both soils and groundwater. For this reason, an accurate representation of plant water use is needed to simulate water and solute transport in large-scale hydrologic and land surface models. In these models, plant water use is frequently estimated by series of equations that rely on many unknown parameters that control characteristics such as rooting depths and how much light the canopy intercepts. Estimating the correct values for these parameters is a challenging task, particularly for distinct plant species in mixed species communities. Our research shows that observations of stable isotopes (^{2}H, ^{18}O) in plant xylem water can be used in model calibration to estimate several plant water-use traits, allowing for more accurate representations of both plants and the water cycle.

1. Introduction

Our capacity to simulate terrestrial water storage, vegetation water use, tree drought mortality risk, and the hydrologic consequences of forest species composition change is dependent on our understanding of soil-water-plant interactions, particularly plant traits influencing rooting strategies, stomatal conductance, and tree water storage (W. R. L. Anderegg, 2015; Feldman et al., 2021; Kannenberg et al., 2022; Konings et al., 2021). Process-based representations of vegetation-water interactions are rapidly improving such that complex plant responses to water stress can be reliably simulated where sufficient empirical data are available to constrain the model parameterizations of vegetation (Berzaghi et al., 2020; Cochard et al., 2021; Fisher et al., 2018; Maneta & Silverman, 2013; Matheny et al., 2017; Mirfenderesgi et al., 2016; Silva et al., 2022; Simeone et al., 2019; Stephens et al., 2021); however, hydrologic characterization of the critical zone (Beyer & Penna, 2021; Goldsmith et al., 2019), measurement of vegetation water contents (Novick et al., 2022), and identification of plant hydraulic traits (L. D. L. Anderegg et al., 2022; Knighton et al., 2021; Matheny et al., 2017) to support such modeling is challenging.

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Isotopes (^{2}H, ^{18}O) in plant xylem water (δ_{XYLEM}) are of particular importance in ecohydrological studies as they support developing reliable estimates of root water uptake (RWU) depth distributions (Beyer et al., 2018; Miguez-Macho & Fan, 2021; Rothfuss & Javaux, 2017), water storage within vegetation (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020), and the partitioning of evapotranspiration into plant transpiration and evaporation from bare soils (Good et al., 2015; Rothfuss et al., 2021). Xylem water isotopic data have strengthened our understanding of biome-scale variations in vegetation water use (Allen et al., 2019; Barbeta & Peñuelas, 2017; Evaristo & McDonnell, 2017; Knighton et al., 2021; Tetzlaff et al., 2021) and subsurface resource partitioning in mixed-species ecosystems (Brum et al., 2019; Gaines et al., 2016; Knighton, Conneely, & Walter, 2019; Knighton, Souter-Kline, et al., 2019; Magh et al., 2020).

Hydrological models that simulate water isotopes in the environment allow for calibration of physical and biological parameters with these novel datasets (Ala-aho et al., 2017; Fekete et al., 2006; Knighton et al., 2017; Kuppel et al., 2018a; Stadnyk et al., 2013). Given that water stored in plant xylem is dependent on stomatal conductance, responses to soil and atmospheric moisture deficits (Gollan et al., 1985), and growth responses to air temperatures, it is likely that, in addition to rooting depths, δ_{XYLEM} observations can inform our understanding of hydraulic traits that govern plant water use. Prior studies have shown some ability to estimate plant traits in the context of process-based model calibration (Kuppel et al., 2018b; Liu et al., 2021; Peaucelle et al., 2019). We therefore hypothesize that ecohydrological and ecological model parameters representing plant hydraulic traits (e.g., maximum stomatal conductance, depth-distribution of roots) are identifiable through calibration of a process-based isotope-enabled model with δ_{XYLEM} data.

Observations of water isotopes in xylem represent the mixture of all water sources taken up by vegetation roots across some representative timescale (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020; Seeger & Weiler, 2021). Observed δ_{XYLEM} is highly variable because of both variations in rooting depths across species (Knighton et al., 2021), and within-species variations which are dependent on local hydrologic conditions (Fan et al., 2017). Field measurement of δ_{XYLEM} is a resource intensive practice (Freyberg et al., 2020), often limiting the temporal frequency and feasible number of trees that can be sampled. Together, these challenges necessitate the assumption that the few xylem observations that have been made in a plot are representative of spatial scales larger than the rooting zones of those individuals or are representative of all individuals of that species (Beyer & Penna, 2021).

A parallel challenge exists in model representations of vegetation where computational and data limitations often prevent the simulation of individual trees, necessitating that the aggregated function of multiple individuals be represented with one set of equations and parameters (Kennedy et al., 2019; Kuppel et al., 2018a; Maneta & Silverman, 2013; Sprenger et al., 2022) (Figure 1). These assumptions are frequently imposed across horizontal grids spanning several meters to thousands of kilometers. How δ_{XYLEM} values of a certain tree species, or across species, can be upscaled to stand- or model grid-scale transpiration fluxes remains an open question.

There have been several recent attempts to use xylem water isotopes for estimation of plant trait values within process-based ecohydrologic models (Brinkmann et al., 2018; Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020; Kuppel et al., 2018b) and StorAge Selection (SAS) function parameters for transpiration (Evaristo et al., 2019; Knighton, Conneely, & Walter, 2019; Knighton, Souter-Kline, et al., 2019; A. A. Smith et al., 2020; Sprenger et al., 2022) through calibration or post-calibration validation. Though each attempted to quantify uncertainty in model parameters related to residuals between simulated and observed δ_{XYLEM}, these studies did not ascertain if the specific trees selected for δ_{XYLEM} sampling were representative of the simulated spatial scale to which they were compared in model calibration.

There have been few attempts to verify that the use of δ_{XYLEM} observations in model parameter estimation is conceptually correct for estimating stand- or catchment-scale transpiration. Comparison of SAS parameter fitting to end-member splitting, young water fractions, and vadose zone observations for the Can Vila catchment in the Spanish Pyrenees mountains suggested that xylem isotopic observations can constrain SAS functions for catchment-scale transpiration, though the difference in scales was noted (Sprenger et al., 2022). Multi-objective calibration of isotope-enabled ecohydrologic models showed that residuals between simulated and observed δ_{XYLEM} and soil moisture isotopic ratios (δ_{SOIL}) were minimized with similar vadose zone parameterizations, suggesting that the processes which dominate vadose zone tracer transport are identifiable by δ_{XYLEM} in some settings (Brinkmann et al., 2018; Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020). In contrast, residuals between δ_{XYLEM} and streamflow showed large tradeoffs, possibly suggesting conceptual limitations
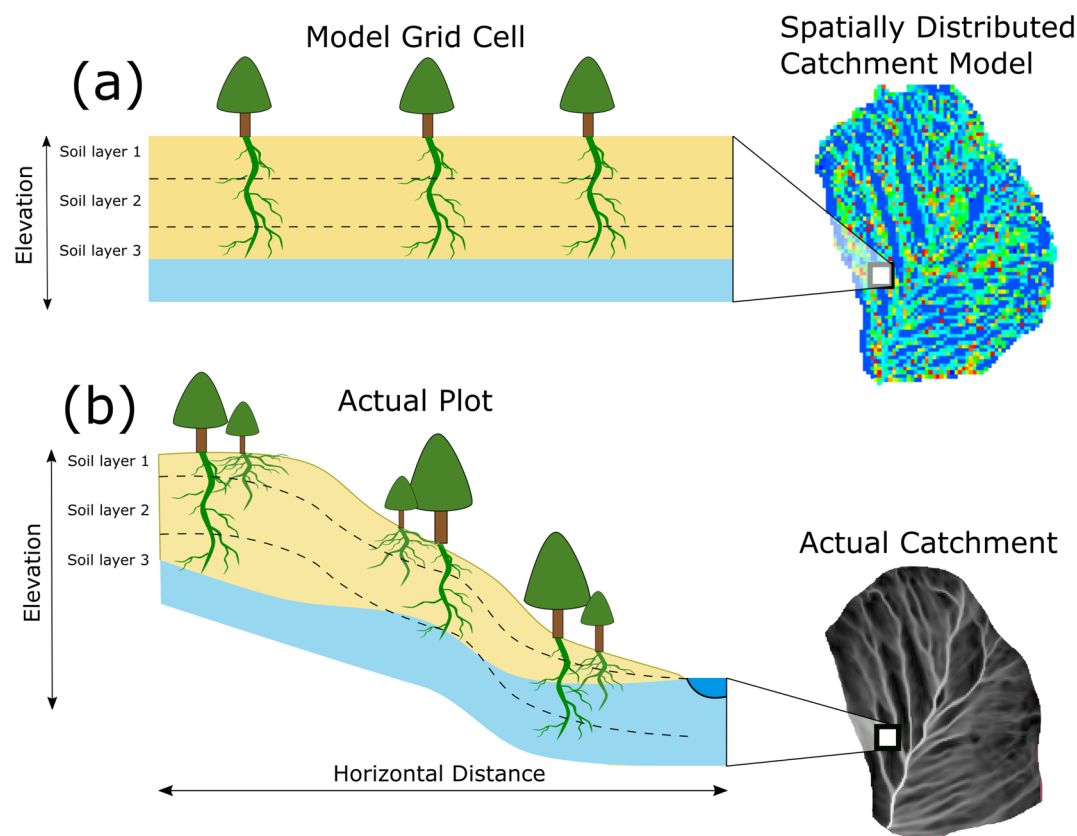
Figure 1. Conceptual diagrams of (a) a numerical hydrological grid cell assuming homogeneous trees and soils and (b) an actual forested plot with trees of varied sizes and topographic positions.

of simultaneously fitting catchment- and plot-scale isotopic and water fluxes (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020). Calibration to continuous in-situ willow isotopic data showed some disagreement between δ_{XYLEM} and δ_{SOIL}, possibly suggesting numerical limitations of the ecohydrological model used (A. Smith et al., 2022). Finally, calibration of a lumped hydrological model to streamflow for 139 forested catchments yielded maximum rooting depths that were correlated with estimates derived from δ_{XYLEM} end member mixing estimates, providing an indirect validation of the use of δ_{XYLEM} as a constraint on rooting depths (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020).

We do not have a strong understanding of the uncertainties introduced to ecohydrological modeling studies by under-sampling vegetation within plots and catchments (Beyer & Penna, 2021; Freyberg et al., 2020; Goldsmith et al., 2019). We will address this knowledge gap by calibrating a plot-scale ecohydrological model to a suite of hydrologic and isotopic measurements, including δ_{XYLEM} observations from 30 eastern hemlock trees, one tree at a time. We hypothesize that ecohydrological model parameters defining vegetation function are correlated with the size and relative topographic position of trees sampled for δ_{XYLEM} used in model calibration (i.e., reflecting traits or positions of individual trees and not that of the stand). We further hypothesize that calibration with δ_{XYLEM} observations from larger diameter trees in a fully grown forest are more representative of the total plot-scale transpiration isotopic composition, which will lead to simultaneous minimization of model residuals for both soil water content and δ_{XYLEM} (i.e., a better overall calibration to measurements in the critical zone).

2. Materials and Methods

2.1. EcH₂O-iso Model Development

We developed a pixel-scale configuration of the study site using the EcH2O-iso model, to examine the information content of δ_{XYLEM} data. EcH₂O-iso simulates the water and energy balance of the landscape as well as

Table 1
EcH2O-iso Model Parameters and Feasible Ranges Considered in Calibration

Parameter	Description	Min	Max	Units
Φ	Porosity	0.4	0.65	$m^3\ m^{-3}$
α	Albedo of bare soil	0.1	0.4	–
λ_{BC}	Brooks-Corey lambda	2	12	–
ψ_{AE}	Soil air entry pressure	0.05	0.8	m
$KH_{SAT}L1$	Saturated horizontal conductivity of layer 1	1.0E−5	0.1	$m^1\ s^{-1}$
$KH_{SAT}L2$	Saturated horizontal conductivity of layer 2	1.0E−5	0.1	$m^1\ s^{-1}$
snow	Snowmelt coefficient	1.0E−10	1.0E−04	m1 K-1
T_{OPT}	Optimal plant growth temperature	15	30	°C
gs_{MAX}	Maximum stomatal conductance	0.001	0.035	$m^1\ s^{-1}$
K_{ROOT}	Root distribution shape parameter	0.01	15	m^{-1}
ψ_D	Limiting matric potential for RWU	100	200	m
TreeV	Tree storage volume for isotopic mixing	1	50	mm
K_{BEERS}	Beer's light extinction coefficient	0.3	0.8	
gs-vpd	Stomatal sensitivity to vapor pressure deficits	1e−5	2e−3	Pa^{-1}
leaf-α	Albedo of vegetation	0.1	0.3	–

tracking water isotopes from precipitation through the canopy, soils, groundwater (Kuppel et al., 2018a; Maneta & Silverman, 2013), and into vegetation (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020).

A coarse grid (1 ha) spatially lumped representation of the study site was chosen (as opposed to a spatially distributed application) to intentionally introduce a mismatch in scales between the measurements collected from individual trees and the simulated transpiration fluxes as this issue is common in the application of ecohydrological and land surface models. All hydrological fluxes are simulated on a daily temporal interval for the period October 2020 through December 2021. The first 5 months of all simulations were discarded as a spin-up. We considered a suite of model parameters related to soil and plant function as calibration parameters (Table 1) based on prior research using this model (Douinot et al., 2019; Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020; Kuppel et al., 2018b; A. Smith et al., 2019).

Soils are represented by three vertically stacked layers with thicknesses of 0.1, 0.2, and 1.2 m (total depth of 1.5 m to the restricting feature). Soil retention and routing are defined by porosity, Φ, and the Brooks-Corey model, characterized by parameters λ_{BC} and ψ_{AE}. Horizontal and vertical hydraulic conductivity are controlled by the horizontal saturated hydraulic conductivity of all three soil layers, $KH_{SAT}L1$, $KH_{SAT}L2$, and $KH_{SAT}L3$, via a vertical-to-horizontal ratio parameter, set to 1 throughout the study. Snow accumulation and melt are controlled by an empirical degree-day melt coefficient, *snow*. Groundwater is drained at the bottom of the soil column based on the *leakance* parameter and the saturated hydraulic conductivity of the deepest layer, $KH_{SAT}L3$, which were held constant at 3.9e−6 $m^1\ s^{-1}$ and 0.025 $m^1\ s^{-1}$ to limit dimensionality. These parameters values were chosen to match the observed groundwater recession rate (presented in Section 5).

Vegetation energy and water use are controlled by the optimal temperature for photosynthesis and above-ground carbon allocation, T_{OPT}, maximum stomatal conductance, gs_{MAX}, exponential decay of depth-distributed of RWU demand, K_{ROOT}, the limiting soil matric potential for RWU, $g_{\psi D}$, stomatal sensitivity to Vapor Pressure Deficits (VPD), *gs*-vpd, and the albedo of vegetation, *leaf*-α (Kuppel et al., 2018b). The fraction of absorbed solar radiation that bypasses the canopy, reaching bare soils, is defined by K_{BEERS}. Xylem water isotopes are solved assuming that each tree is a well-mixed reservoir with some volume *TreeV*. Prior research supports this approach as it is more appropriate than assuming the simulated isotopic composition of RWU is equivalent to that of tree-stored water during periods of low transpiration (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020).

2.2. Model Parameter Sensitivity Analysis and Multi-Objective Model Calibration

We performed 20,000 simulations where each parameter was randomly sampled with uniform distributions defined by the feasible ranges in Table 1. The sensitivity of model predictions of water volumes and soil and xylem water isotopes to parameter values was determined with the multi-objective generalized sensitivity analysis (MOGSA) algorithm (Bastidas et al., 1999). We tested for both global pareto sensitivity as well as single-objective sensitivity to each calibration data set. With this and all subsequent hypothesis tests, we evaluated significance at the σ thresholds of 0.1, 0.05, and 0.01.

Model calibration was performed with an approach similar to that of the Generalized Likelihood Uncertainty Estimation approach (Beven & Binley, 2014). The Root Mean Square Error (RMSE) was calculated between each simulation and the observed volumetric water content (VWC) and δ_{SOIL} for all three soil layers (median values across all three soil profiles in each soil layer for each sampling day), groundwater depth, δ_{GW}, and the δ_{XYLEM} of each of the 30 trees. Only δ^{18}O data was used in calibration to limit uncertainty related to the potential for δ^2H biases in plant water extraction (Allen & Kirchner, 2021; Chen et al., 2020). As will be demonstrated, substantial model performance tradeoffs exist between accurate simulation of VWC of soil layer 1 (VWC L1) and δ_{XYLEM} (possibly attributable to model formulation, discretization, or non-representation forcing or calibration data). We therefore define the "accepted" parameter sets as those resulting from simulations that defined the Pareto frontier (i.e., all non-dominated simulations) between VWC of soil layer 1 and δ_{XYLEM}. This process was repeated for each of the δ_{XYLEM} observations from the 30 sampled trees, resulting in 30 different sets of accepted parameter values. We compared the median of pareto optimal ecohydrological parameter values to estimates derived from independent field studies. To explore the impact of soil profile heterogeneity, this calibration exercise was repeated three times with data from the three soil profiles separately (Section S4 in Supporting Information S1).

2.3. Independent Estimation of Vegetation and Soil Parameters

We estimated the values of hemlock vegetation parameters (maximum stomatal conductance [gs_{MAX}], stomatal sensitivity to VPD [gs-VPD], canopy light extinction coefficient, [K_{BEERS}], and the depth distribution of roots, K_{ROOT}, and tree water storage, [$TreeV$]) from independent empirical datasets collected at other research sites. We estimated the parameters gs_{MAX} and gs-VPD with observed daily Latent Energy flux (LE) from the Harvard Forest Eastern Hemlock site, comprised of 83% hemlock, for 2004–2011 (Hadley & Munger, 2022). Data after 2012 was not used to estimate the parameters due to an insect outbreak which significantly altered stand water use (Kim et al., 2017). Both parameters were estimated with a Penman-Monteith (P-M) model accounting for stomatal closure in response to VPD (Maneta & Silverman, 2013). Records with incomplete climate or LE data were discarded from analysis. The effect of soil moisture limitations on stomatal conductance and LE were not simulated due to the lack of available soil moisture observations. Model parameters were randomly sampled 20,000 times within the ranges of Table 1. We accepted the parameter set producing the maximum Nash Sutcliffe Efficiency (NSE) between observed and simulated daily LE. An estimate of K_{ROOT} was derived from end member mixing analysis of δ_{XYLEM} and δ_{SOIL} observations from a riparian hemlock stand in the Hammond Hill Research Catchment (HHRC) (Knighton, Conneely, & Walter, 2019; Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020; Knighton, Souter-Kline, et al., 2019). K_{BEERS} was estimated from measurements of canopy openness in several hemlock stands across North America (Lefrançois et al., 2008). TreeV was estimated based on prior sampling of hemlock in a nearby temperate catchment (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020). For a full description of hemlock parameter estimates see Section S1 in Supporting Information S1.

The soil parameters of porosity, ϕ, and the Brooks & Corey parameters air entrainment, Ψ_{AE}, and lambda coefficient, λ_{BC}, were estimated from soil textures and published properties (Dingman, 2015).

2.4. Impact of Tree Selection on Model Parameter Estimation

We tested if EcH$_2$O-iso calibrated model parameters related to plant water use and growth exhibit significant ranked correlations with tree diameter at breast height (DBH) or horizontal distance from the stream bank edge, with Kendall's coefficient (τ), a metric that quantifies the degree of rank correlation between two vectors. We then tested if data from trees with certain characteristics produced more representative calibrations by comparing
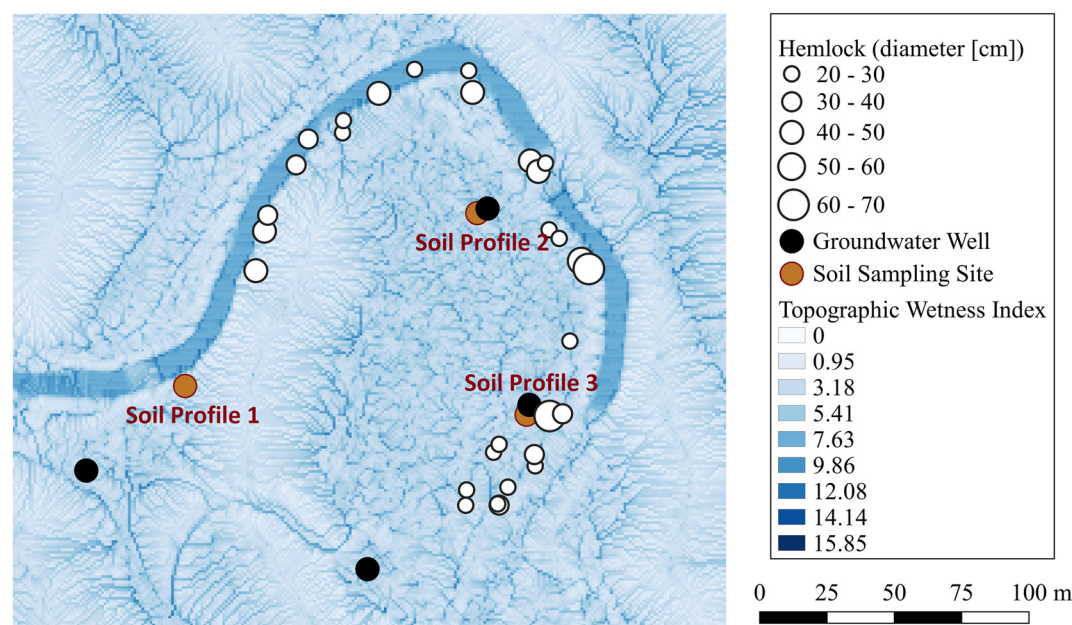
Figure 2. Topographic wetness index (TWI) map showing sampling locations of groundwater, soil moisture, and the 30 individual hemlock trees sampled for δ_{XYLEM}.

correlations between two objective functions, RMSE(δ_{XYLEM}) and RMSE (VWC L1), and tree DBH or horizontal distance from the stream bank edge with Kendall's coefficient (τ).

3. Site Description and Ecohydrological Measurements

Ecohydrological measurements and samples were collected along a riparian corridor of the University of Connecticut forest. The sampling area was approximately 1 ha (Figure 2), comparable to the horizontal grid scale of distributed hydrologic and land surface models. The study area has a mean annual precipitation of 1,410 mm, and a mean annual temperature of 9.7°C (NOAA, 2022). Soils to 1 m depth are a uniform well-drained fine sandy loam (Natural Resources Conservation Service, 2022). The forest cover is dominated by Eastern hemlock (Tsuga canadensis) with a basal area of 1.03 m^2 ha^{-1} (Li & Knighton, 2022).

Meteorological conditions were recorded 3.2 km from the study site. Groundwater elevations were recorded from May through December at a 15-min interval with a pressure transducer at a well installed at the center of the plot. Soil Gravimetric Water Content was measured for discrete soil samples collected at a monthly interval at depths of 5, 10, 20, 30, 40, and 50 cm. Soil VWC depth profiles were estimated from VWC measurements and validated with soil moisture measurements taken of the upper 10 cm with a handheld probe (Campbell Scientific, CS620).

We measured the isotopic composition (^{2}H, ^{18}O) of precipitation, stream water, groundwater, soil moisture (three profiles), and the xylem water of 30 hemlock trees. Precipitation was collected at a daily interval (when present) in a glass jar with a funnel and plastic ball to prevent evaporation. Groundwater wells and streamwater were sampled at a monthly interval. Bulk soil samples were collected in triplicate at 5, 10, 20, 30, 40, and 50 cm (above which 90% of roots were found) with an auger at a monthly interval. Tree cores were sampled at breast height with an increment borer at a monthly interval to a depth that spanned the sapwood of each tree. Hemlock trees ranged in DBH from 20 to 68 cm, in elevation from 90 to 103 m MSL, and in distance from the stream from 0 to 31 m. Elevation and horizontal distance of hemlock are significantly correlated.

Water from soil and tree core samples were extracted via Cryogenic Vacuum Extraction for a minimum of 60 min at a pressure of 0.2 kPa and a temperature differential of 200°C on a system built following specifications in Orlowski et al. (2013). All water samples were analyzed for δ^2H and δ^{18}O on a Picarro L-2130i. All samples were run with three standards exceeding the range of measurements collected and screened for organic contamination. Further details on field sampling and lab analysis are documented (Li & Knighton, 2022). All precipitation,
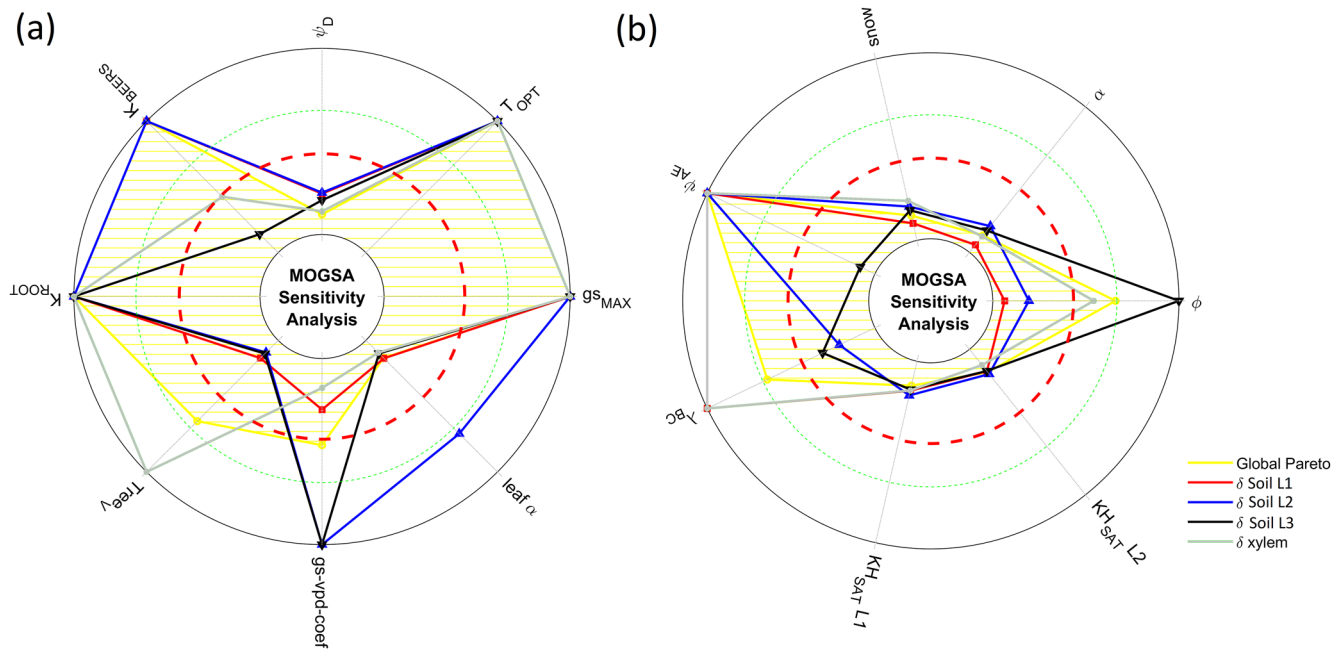
Figure 3. Multi-objective Generalized Sensitivity Analysis (MOGSA) of EcH$_2$O-iso simulated soil and xylem water isotopic data with respect to (a) vegetation and (b) soil parameters. The alpha thresholds of 0.1, 0.05, and 0.01 are shown with red, green, and black lines respectively.

groundwater, soil, and xylem water isotopic data used in this study are publicly available (Knighton, 2022). Groundwater isotopes were averaged across all wells for each sampling day. Soil VWC and moisture isotopic values were computed as the median value for each soil layer (across the three sampling locations) for each date.

4. Results

4.1. Independent Estimation of Hemlock Vegetation Parameters

The P-M model calibrated to LE flux from the Harvard Forest Hemlock Site produced a daily NSE value of 0.47 and P-Bias of +0.4% (Figures S1, S2a, and S2b in Supporting Information S1). The simulated and observed regressions of LE and VPD were similar, though with less variance in the simulated LE response (Figure S2c in Supporting Information S1). The underlying relationship between stomatal conductance (gs) and VPD suggests stomatal closure in response to increasing VPD (Figure S2d in Supporting Information S1). We estimated gs_{MAX} and gs-VPD to be 9.7e−3 m^1 s^{-1} and 3.3e−4 Pa^{-1}, respectively. The flux tower derived gs_{MAX} was slightly higher than observed maximum midday gs in August (Domec et al., 2013).

The value of K_{ROOT} was estimated to be 4.58 m^{-1} with xylem and soil water isotopic data collected from a riparian site in the HHRC (Knighton, Conneely, & Walter, 2019; Knighton, Souter-Kline, et al., 2019). The value of K_{BEERS} was estimated to be 0.495 with hemlock canopy openness measurements collected at several hemlock stands across North America (Lefrançois et al., 2008).

4.2. Model Parameter Sensitivity Analysis

EcH$_2$O-iso simulation of vadose zone isotopic fluxes demonstrated significant global Pareto sensitivity to several plant (K_{ROOT}, gs_{MAX}, T_{OPT}, K_{BEERS}) (Figure 3a) and soil (Φ, ψ_{AE}) (Figure 3b) parameters at the p-value < 0.01 threshold. Several other parameters were globally sensitive at the p-value < 0.05 threshold ($TreeV$, gs-vpd, λ_{BC}). Our subsequent research questions therefore focus on those parameters to which the model demonstrated significant global sensitivity (K_{ROOT}, $TreeV$, gs_{MAX}, gs-vpd, T_{OPT}, K_{BEERS}, Φ, ψ_{AE}, and λ_{BC}).

Single objective sensitivity to δ_{XYLEM} data alone demonstrated that the values of 5 vegetation parameters (Figure 3a) and 3 soil parameters (Figure 3b) induced significant responses at the p-value < 0.05 threshold. The sensitivity of δ_{XYLEM} residuals to parameter values was redundant to that of δ_{SOILS} for gs_{MAX}, T_{OPT}, K_{BEERS}, K_{ROOT},
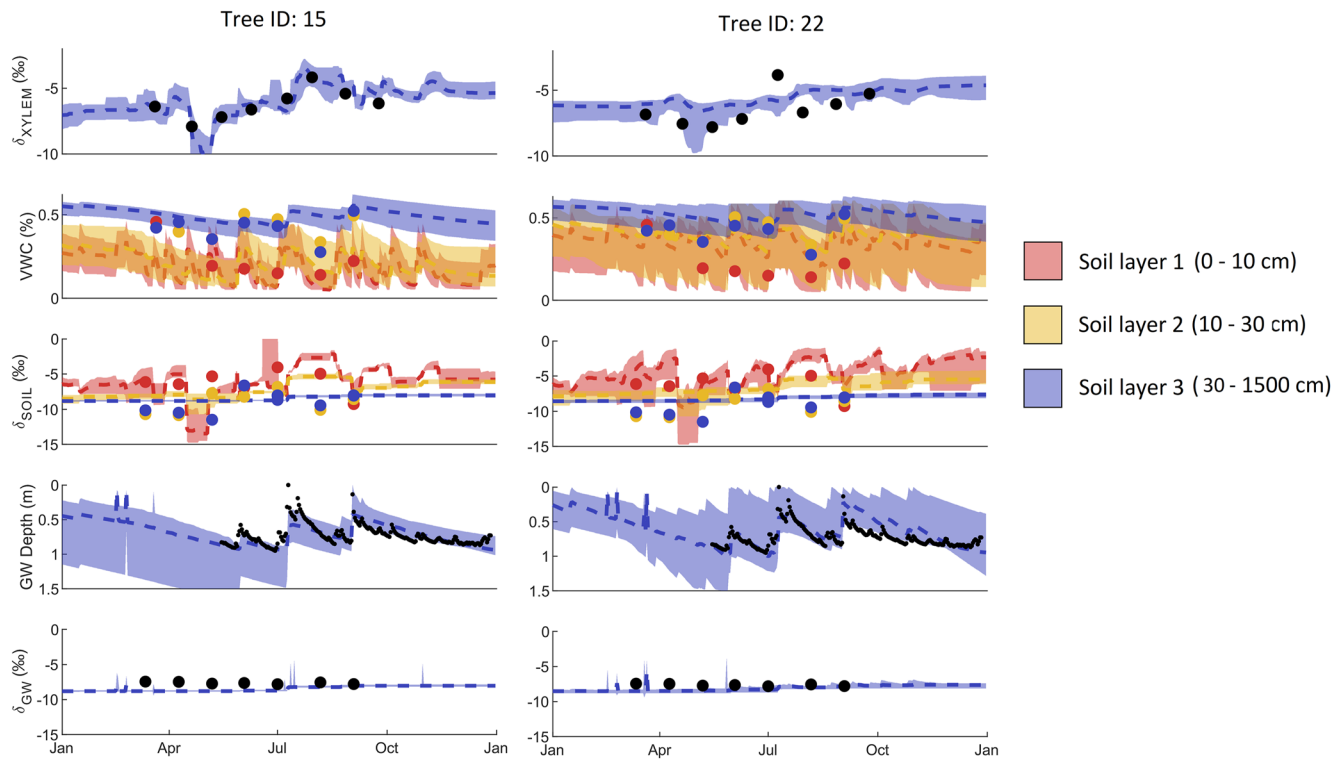
Figure 4. Model predictions for the pareto optimal parameter sets of the best (Tree ID 15) and worst (Tree ID 22) δ_{XYLEM} calibrations, showing 95% confidence intervals (shaded), median predictions (dashed lines), and observations (dots).

Φ, and ψ_{AE}, and unique for *TreeV* and λ_{BC}. Calibration to soil VWC measurements indicated sensitivity to fewer model parameters (Figure S3 in Supporting Information S1).

4.3. Multi-Objective Parameter Estimation

The strongest calibration tradeoffs as measured by the variance in δ_{XYLEM} RMSE occurred between δ_{XYLEM} and the VWC of the uppermost soil layer (Figure S4 in Supporting Information S1). We therefore defined "accepted" model parameter sets as those simulations defining the pareto front between δ_{XYLEM} and the VWC of the uppermost soil layer (VWC L1) (Figure S4 in Supporting Information S1). This definition encompasses a large range of uncertainty in model parameter values and provides reasonable representations of ecohydrological fluxes in all simulated compartments (Figure 4). The remaining hydrologic and isotopic observations including soil VWC from deeper soil layers (>10 cm) was used to provide a validation of the model parameterization. Both calibrations demonstrated tradeoffs between the minimization of residuals for δ_{XYLEM}, soil VWC, and δ_{SOILS} from all three layers (Figure 4 and Figure S4 in Supporting Information S1). Calibration was performed with both the median of the measured soil profiles (Figures 5 and 7) and for each of the profiles separately (Figures S5, S6, and S7 in Supporting Information S1) to explore the role of soil heterogeneity on plant trait identification. All analyses returned comparable plant trait values and relationships to tree characteristics. Further details are presented in Section S4 in Supporting Information S1.

We observed relatively low variance in calibrated maximum stomatal conductance, gs_{MAX}, optimal growth temperature, T_{OPT}, Beer-Lambert canopy radiation interception parameter, K_{BEERS}, depth distribution of RWU, K_{ROOT}, and stomatal sensitivity to VPD, gs-vpd, across all trees relative to the feasible ranges (Figure 6, Table 1). The volume of tree water storage that RWU mixes into, *TreeV*, showed substantial tree-to-tree variations (Figure 6).

The median of calibrated gs_{MAX} values across all trees, 0.0099 m^1 s^{-1}, was similar to the value derived from flux tower data from the Harvard Forest hemlock site, 0.0097 m^1 s^{-1} (Figure 5). The median calibrated K_{BEERS}, 0.44, was similar to the value derived from observations of hemlock canopy openness, 0.495 (Lefrançois et al., 2008). The median calibrated K_{ROOT}, 4.65 m^{-1} was similar to the value estimated for a riparian hemlock stand at the
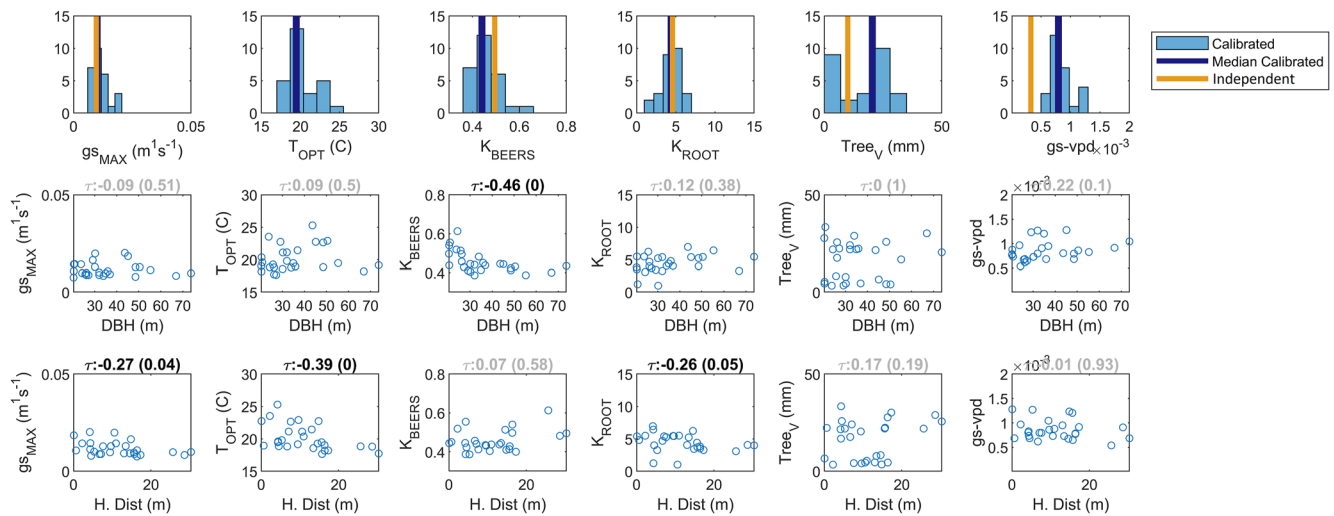
Figure 5. Histograms of calibrated plant parameters, showing the median across all trees (blue line) and trait values derived from independent datasets (orange line), and correlations with diameter at breast height and horizontal distance from the stream, showing Kendall's τ and p-values in parentheses.

HHRC, 4.58 m^{-1} (Knighton, Conneely, & Walter, 2019; Knighton, Souter-Kline, et al., 2019) and also in agreement with broad conclusions derived from hemlock needle δ^2H analysis at this riparian site (Oakes & Hren, 2016).

We observed disagreement in estimates of hemlock stomatal responses to VPD. The median gs-VPD estimate derived from δ_{XYLEM} with EcH$_2$O-iso, 7.5e−4, suggested a higher degree of stomatal closure in response to increasing VPD than was estimated from at the Harvard Forest Hemlock Site, 3e−4 (Figure S2 in Supporting Information S1 and Figure 5). There is less certainty around the accuracy of tree water storage volume, *TreeV*, estimates. The median calibrated internal volume of hemlock trees was 24 mm, less than that estimated for hemlock using xylem isotopic measurements in the context of EcH2O-iso calibration at the HHRC$_2$, 50 mm (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020), but greater than a volume of 9.4 mm estimated for another conifer, Scots Pine (*Pinus sylvestris* L.), using deuterium tracers (Urban et al., 2015).

Several significant correlations between tree characteristics and calibrated trait values were observed (Figure 5). Maximum stomatal conductance, gs_{MAX}, was negatively correlated with tree horizontal distance from the stream, suggesting higher conductance in riparian hemlock. The optimal growth temperature, T_{OPT}, was significantly negatively correlated with distance from stream, suggesting that further upslope trees had lower optimal growth temperatures. The Beer-Lambert light extinction coefficient, K_{BEERS}, was significantly negatively correlated with DBH, suggesting smaller diameter trees absorbed more solar radiation per unit area. The rooting parameter, K_{ROOT}, tree water storage volume, *TreeV*, and stomatal sensitivity to VPD, gs-VPD, were not significantly correlated with any measured tree characteristics.

Significant rank correlations exist among several plant parameter values. Higher optimal growth temperatures are observed in trees with higher gs_{MAX}, shallower roots (higher K_{ROOT}), lower *TreeV*, and higher gs-VPD (Figure 6). Trees with higher gs_{MAX} also exhibited lower *TreeV* (Figure 6).

Calibrated parameters describing soil-water interactions showed minimal variations (Figure 7). Calibrated values for both soil porosity, Φ, and the Brooks-Corey air entrainment parameter, Ψ_{AE}, deviated from expected values for sandy-loam soils (Figure 7), whereas the Brooks Corey shape parameter, λ_{BC}, agreed with expected values. Calibrated Φ values were positively correlated with DBH, and λ_{BC} was negatively correlated with tree distance from the stream, though we note that the variances of calibrated values were minimal.

We examined the relationships between tree characteristics and the RMSE of δ_{XYLEM} and the RMSE of soil VWC L1 (Figure 8). There were no significant correlations between tree characteristics and RMSE of δ_{XYLEM}. Root Mean Square Error for soil VWC L1 was significantly correlated with tree size, where calibration to smaller diameter trees provided the best simulations of shallow soil water contents in contrast with our hypothesis.
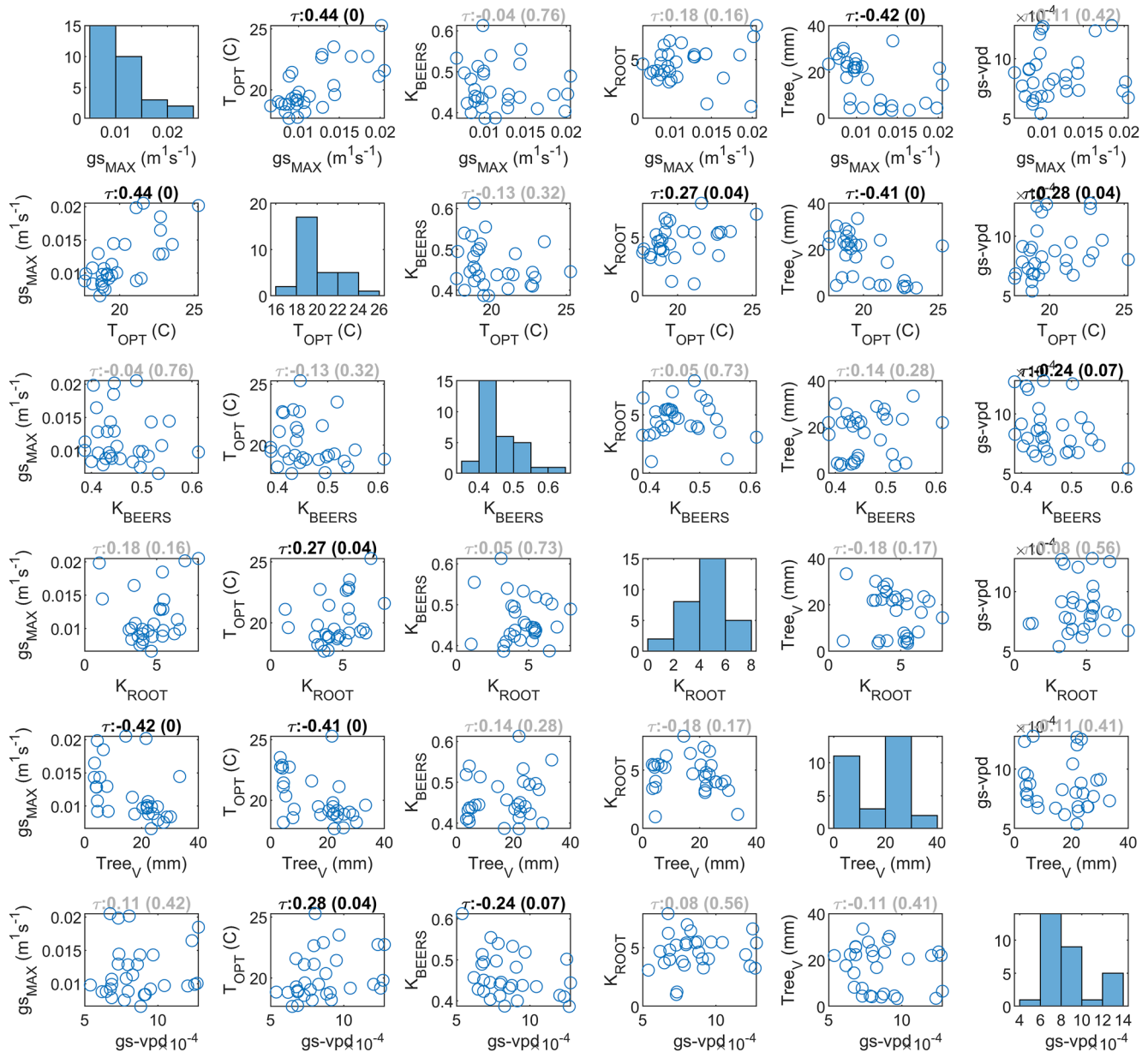
Figure 6. Correlations between plant parameters estimated for 30 hemlock trees, showing Kendall's τ and p-values in parentheses.

5. Discussion

5.1. Plant Trait Estimation From δ_{XYLEM} Observations

The EcH$_2$O-iso estimate of gs_{MAX} agreed with values derived from flux tower LE (Figure 5) but was larger than field-observed gs (Domec et al., 2013), possibly suggesting the measured midday August stomatal conductance was limited by low soil moisture or high VPD. We also note that the independent estimate of gs_{MAX} could have been a slight underestimate caused by the assumption of a non-limiting soil water supply.

Calibrated and observed K_{BEERS} values indicated that canopy shading is identifiable by δ_{XYLEM} data, likely because of the effect of solar radiation interception driving the partitioning of evaporation and transpiration. EcH$_2$O-iso simulates evaporative fractionation due to evaporation from bare soils and assumes no fractionation at RWU (Kuppel et al., 2018a). K_{BEERS} influences δ_{SOILS} and δ_{XYLEM} more significantly than it does soil moisture (Figure 3 and Figure S3 in Supporting Information S1), highlighting the value of using both water quantity and
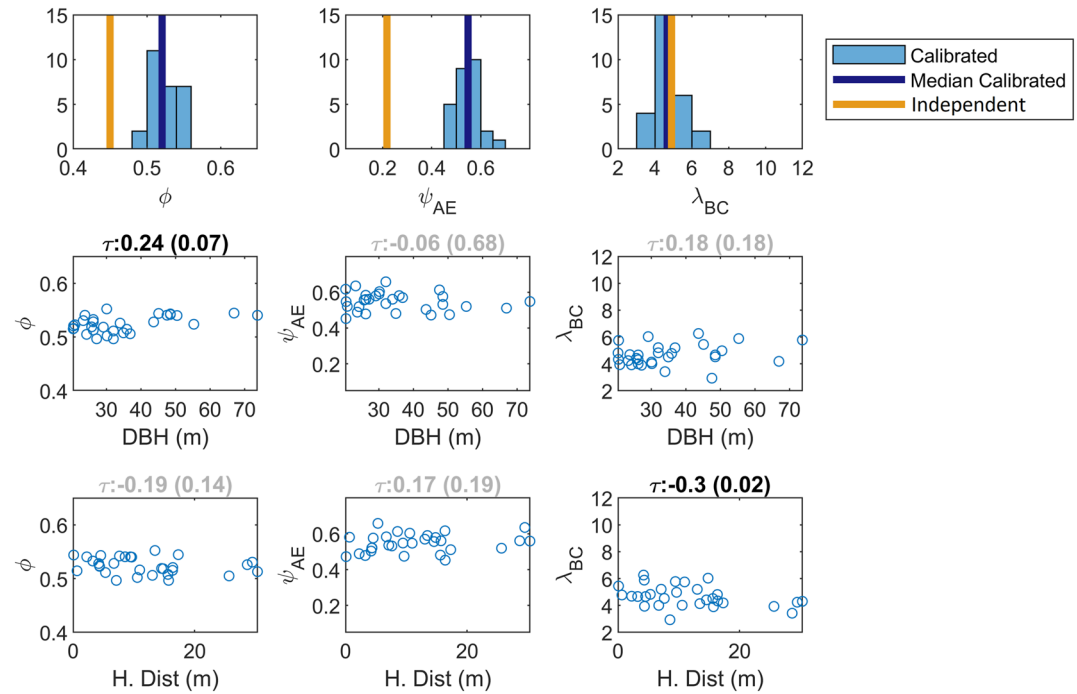
Figure 7. Histograms of calibrated soil parameters, showing the median across all trees (blue line) and trait values derived from independent datasets (orange line), and correlations with diameter at breast height and horizontal distance from the stream, showing Kendall's τ and p-values in parentheses.

water isotopic data. Our observation of a negative correlation between K_{BEERS} and DBH is in agreement with the observation that canopy openness is positively correlated with hemlock DBH (Lefrançois et al., 2008).

Calibrated hemlock water uptake depths were similar to both prior end member mixing analyses (Knighton, Conneely, & Walter, 2019; Knighton, Souter-Kline, et al., 2019) and process-based model calibration exercises (Knighton et al., 2017; Knighton, Conneely, & Walter, 2019; Knighton, Souter-Kline, et al., 2019) centered on a hemlock stand in a nearby catchment. Both δ_{XYLEM} datasets indicated that approximately 2/3 of hemlock-transpired water was taken up by roots from the shallowest 30 cm of soils during the summer season. This finding is also in general agreement with observations of a reliance on shallow water uptake by conifers (Allen et al., 2019; Knighton et al., 2021). The lack of a significant correlation between K_{ROOT} and DBH conflicts with empirical
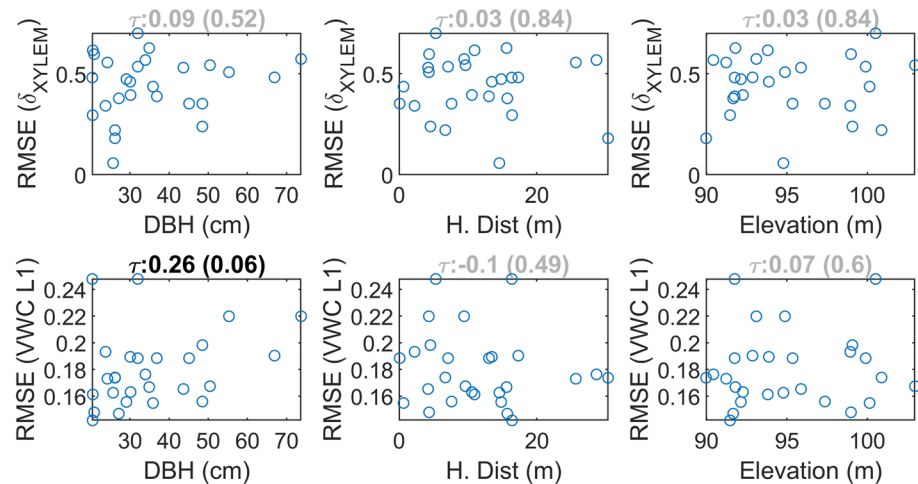

Figure 8. Correlations between calibration objective functions (δ_{XYLEM}, δ_{SOILS}) and tree characteristics.

analysis of this data set (Li & Knighton, 2022). Numerical solutions of the land surface energy balance within EcH$_2$O-iso are improved with thicker soil layers that can hold larger volumes of water. The requirement of soil layer thickness likely obscured DBH-related variations in water uptake that were previously identified across the upper 20 cm (Li & Knighton, 2022).

There was some disagreement between the two estimates of *gs*-VPD. Hemlock transpiration rates exhibited a linear relationship between VPD and LE (Figure S2c in Supporting Information S1) similar to observed hemlock leaf-scale stomatal conductance (Ford & Vose, 2007). An EcH$_2$O-iso *gs*-VPD value of 3e−4 reproduces this linear relationship (Figure S2c in Supporting Information S1), whereas the calibrated value of 7.5e−4 results in a non-linear relationship with a substantial reduction in LE at high VPD. These comparisons suggest that the *gs*-VPD values estimated from calibration to δ_{XYLEM} are not reliable with the current formulation of the model. Poor identification of *gs*-VPD through EcH$_2$O-iso calibration δ_{XYLEM} is possibly the result of an overcorrection for misidentified soil parameters which influence soil moisture tensions, and therefore transpiration rates (Figure 7). Further, this discrepancy may translate controls of missing processes such as tree column hydraulics, as this version of the EcH$_2$O-iso model assumes that leaf water potential equals soil water potential in the root zone (Maneta & Silverman, 2013). Therefore, plant-scale conductance during drier (higher VPD) conditions may be limited by root-to-shoot water transport in addition to stomatal regulation, and further analysis may benefit from tree hydraulics developments in the original EcH$_2$O model, provided that the associated parametrization can be appropriately constrained (Simeone et al., 2019). Alternatively, the disagreement may reflect the reduced sensitivity to *gs*-VPD than other parameters which may have dominated the multi-objective calibration (Figure 5).

Above-ground water storage, *TreeV*, was only sensitive to δ_{XYLEM} and not to any measurements made within the soils (Figure 3 and Figure S3 in Supporting Information S1). The simulation of above-ground water storage in vegetation is a developing front that is enabling studies of plant drought stress, xylem embolism, and conductance recovery (Liu et al., 2021; Mencuccini et al., 2019; Mirfenderesgi et al., 2016; Niu et al., 2020). Stand-representative δ_{XYLEM} data could be a critical tool to advance the development of species-level representations of vegetation in process-based ecohydrological models; however, further research is required to understand water transport within vegetation and the impact on δ_{XYLEM} (De Deurwaerder et al., 2020; Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020; Seeger & Weiler, 2021). Empirical measurements of vegetation water content and stem water potentials support more accurate simulation of whole-plant stomatal conductance (Simeone et al., 2019). A wider availability of such measurements would support the inclusion and validation of these processes in species-level ecological and hydrological model simulations across broader regions.

Our finding that constraining a process-based model with hydrologic flux data can yield ecologically consistent vegetation parameter values is in agreement with other recent work (Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020; Kuppel et al., 2018a; Liu et al., 2021; Peaucelle et al., 2019). Model sensitivity analysis further indicated that δ_{XYLEM} data can support estimation of plant trait values related to rooting, stomatal conductance, growth temperatures, and possibly tree water storage (Figure 3). Isotopic tracer data provided stronger feedbacks on model parameter values than soil water content observations (Figure 3 and Figure S3 in Supporting Information S1). This approach could facilitate species-level simulations to close a substantial knowledge gap needed to study the differential impacts of drought and forest composition change in mixed-species forests.

Estimates of whole-ecosystem vegetation phenology and water use have also been derived from remotely sensed observations (Liu et al., 2021). Though recent progress supports possible identification of individual species in mixed-species stands (Mäyrä et al., 2021; Onishi & Ise, 2021; Schiefer et al., 2020), widely available vegetation index products (e.g., Normalized Difference Vegetation Index (NDVI), Vegetation Optical Depth (VOD)) may accurately support trait estimation for distinct species in mixed stands (Didan, 2015; Moesinger et al., 2020). Phylogenetic models can potentially predict traits from the underlying genetic relationships among plants; however, these methods are largely unvalidated (L. D. L. Anderegg et al., 2022; Knighton et al., 2021). New methods of estimating plant hydraulic traits could remove a significant barrier to progress in the study and simulation of soil-water-plant interactions. Plant xylem water isotopic data exists for a substantial number of tree species, although sampling frequency greatly vary across studies (Barbeta & Peñuelas, 2017; Evaristo & McDonnell, 2017) and observational uncertainties have been highlighted in various cases (Millar et al., 2022). Nonetheless, datasets containing enough points to infer intra-seasonal dynamics hold significant potential for use with process-based models to estimate plant traits.

5.2. Impact of Tree Selection on Vegetation Parameterization

Despite δ_{XYLEM} providing a similarly strong constraint on model parameter values to δ_{SOIL} as estimated via MOGSA (Figure 3), variations in calibrated parameter values indicated that field observed δ_{XYLEM} from individual trees were not necessarily valid approximations of transpiration across the entire stand (Figure 5). Correlations between tree size, topographic position, and calibrated trait values demonstrated that δ_{XYLEM} data reflect the ecohydrological characteristics and fluxes occurring within the specific trees that are sampled. Observations of δ_{XYLEM} inform us only on soil-water processes within the vicinity of the plant's roots and also likely reflect characteristics of the individual plant that has been sampled (e.g., species identity, topographic position, rooting structure, stomatal conductance, sensitivity to air temperature, phenology) (Gaines et al., 2016; Knighton, Conneely, & Walter, 2019; Knighton, Souter-Kline, et al., 2019; Li & Knighton, 2022; Snelgrove et al., 2021). These observed correlations between vegetation parameters, DBH, and topographic position (Figure 5) can possibly support new scaling relationships to better simulate spatial variations of vegetation function where empirical measurements would be infeasible and global long-term remotely-sensed vegetation indices possibly too coarse. The lack of anticipated significant correlations between DBH and *TreeV* possibly suggest that more complex model representations of tree water storage and transport are required.

We observed no significant ranked correlations between RMSE of δ_{XYLEM} and tree characteristics, but significant improvements in model skill at simulating soil moisture when data from smaller diameter trees was used (Figure 8). The improved calibration to smaller trees conflicts with our initial hypothesis. This result can possibly be explained by smaller diameter trees representing a greater fraction of transpiration than large diameter trees. Another explanation is that the collected soil data were most representative of conditions around the small diameter trees in this sampling plot; however, our analysis suggests that this result is possibly less likely (Figures S5, S6, and S7 in Supporting Information S1).

The environmental water isotopic heterogeneity of soils and vegetation tends to be high (Beyer & Penna, 2021). Field designs frequently rely on random selection of sampling locations to minimize spatial bias in sampling. Our calibration results possibly suggest that field sampling procedures could be designed with consideration for representative vegetation soil and vegetation to minimize the bias in up-scaling from individual trees and soil pits to the stand. The observed correlations among calibrated plant parameter values (Figure 6) also possibly suggest that model dimensionality could be reduced through use of transfer functions.

Further research may benefit from exploring relationships between model fits to δ_{XYLEM} and plant measurements that can possibly characterize plant water use strategies including transpiration rates, plant water potentials, leaf area indices, or UAV-based vegetation indices such as NDVI or VOD (Kannenberg et al., 2022; Konings et al., 2021; Moesinger et al., 2020).

5.3. Multi-Objective Calibration Tradeoffs in the Critical Zone

Discrepancies between expected and calibrated soil physical properties (Figure 7) and imperfect reproduction of all observed data (Figure 4) indicated some limitations of multi-objective model fitting to critical zone water and isotopic fluxes. A challenge in the use of process-based ecohydrological models for plant source water identification is the need to define the parameters controlling the boundary condition on RWU (e.g., soil moisture content, groundwater elevation). If we assume that any model is a strong representation of the biophysical system and all boundary conditions are well defined (i.e., accurate meteorological forcing data), model parameterizations that minimize residuals of δ_{XYLEM} should also minimize residuals of all other hydrological fluxes and stores (e.g., soil moisture contents, δ_{SOILS}, groundwater recharge). This result has been realized in several prior case studies (Brinkmann et al., 2018; Knighton, Kuppel, et al., 2020; Knighton, Singh, & Evaristo, 2020); however, this study found strong tradeoffs between δ_{XYLEM} and other measured hydrologic variables (Figure S4 in Supporting Information S1).

The reasons for these calibration tradeoffs may be grouped into three classes for the model-data approach presented here. First are the uncertainties associated to the forcing data itself. Second is the effective leverage of the calibration data, as the propagated information content varies in terms of process-level or spatio-temporal "footprint" brought by each data set (e.g., Kuppel et al., 2018b), some being sensitive to spatial under-sampling. Third is the structural model uncertainty stemming from numerical over-simplifications of the simulated system. Among those are the model horizontal scale being larger than the spatial scale of observations; the number of soil

layers (3) limiting the description of horizon-based hydrodynamics; a fixed root profile which limits the extent of temporally varying uptake profile, although its shape may depend on storage status and water table fluctuations (Fan et al., 2017); the absence of explicit tree hydraulics, whereby leaf water potential currently reflects soil water potential in the model (Simeone et al., 2019); simplified representations of xylem water storage and mixing; and the assumptions that no fractionation occurs during soil-to-stem water transit.

6. Conclusions

Accurate modeling of terrestrial water fluxes is critical for solving water resources challenges under both present-day and anticipated climate conditions. New experiments are needed to estimate plant traits related to water use to simulate the responses of ecosystems, terrestrial water stores, transpiration, and streamflow to external climate stressors. A major challenge to species-level representation of vegetation is our lack of knowledge of reasonable parameters for trees that have not previously been the focus of extensive empirical research. We demonstrated that accurate estimates of several Eastern hemlock traits related to water use could be retrieved by calibrating a process-based ecohydrological model with tree xylem water isotopic data. We observed that the calibrated values for several traits were significantly correlated with tree diameters and topographic positions suggesting that trait values estimated for individual trees may not always be an appropriate representation of vegetation across larger horizontal scales. These conclusions suggest that care must be taken when integrating trait values derived from xylem water isotopic calibration into large-scale ecohydrological and ecosystem models.

Data Availability Statement

Model Code Availability: EcH2O-iso is an open-source ecohydrological model (https://bitbucket.org/scicirc/ech2o-iso), with the version used in the study available from https://doi.org/10.5281/zenodo.7299207 (Kuppel, 2022). *Observational Data Availability*: The field campaign data used for this research are publicly available on HydroShare—Fenton Tract Forest Research http://www.hydroshare.org/resource/8996065d-3ba34907a018be9b4369c1d3 (Knighton, 2022).

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