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Modelling temporal variability of in situ soil water and vegetation isotopes reveals ecohydrological couplings in a riparian willow plot

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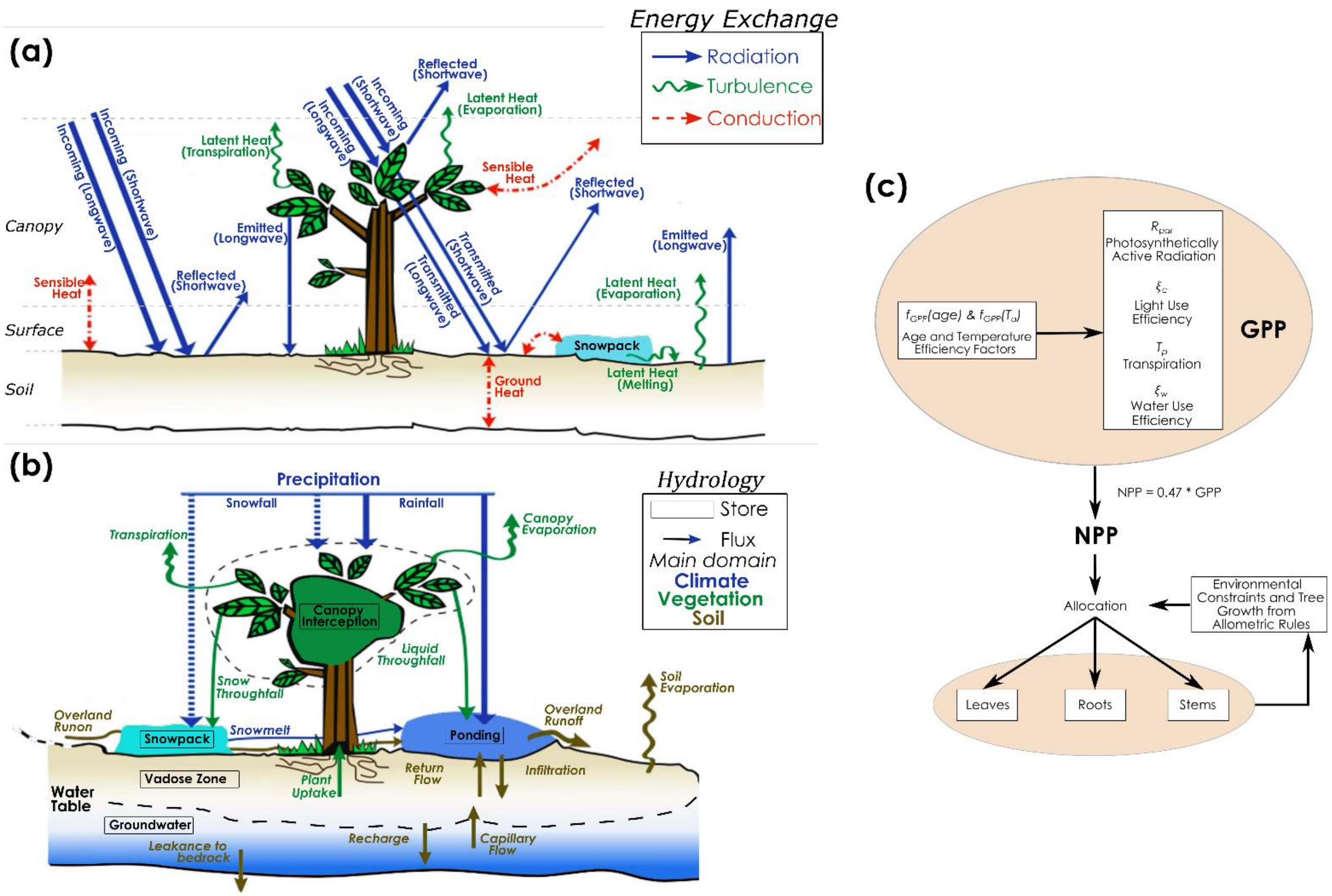


Figure S1: Conceptual diagram of the (a) energy and (b) water balance within EcH$_2$O-iso, and the (c) carbon uptake and allocation within vegetation to roots, stem, and leaves. Modified from Smith et al., 2020 and Maneta, 2021.

Text S1: Detailed Description of In-situ Measurements

Destructive Sampling

Replicate samples of soil isotopes were collected monthly (June – Oct) using bulk soil water sampling with a soil auger. Samples were taken at increments of 0-10, 10-20, 20-40, 40-70, and 70-100cm. Samples were sealed in a metalized bag, equilibrated from 48hours prior to analysis. Analysis was conducted using the direct-equilibrium method from Wassenaar et al., (2008) and described in more detail for the IGB laboratory in Kleine et al. (2020). Correction of water samples included nine 10ml standard samples 18O (-10.3, -7.68, 2.91 or 1.53‰) and 2H (-72.81, -56.70, 0.78 or 16.74‰), utilized for all sampling periods.

Destructive vegetation samples were conducted monthly (July – Oct) using samples from three (unique) sun-exposed branches on each willow tree. Only branches where bark was unimpaired were sampled. Collected branches had the bark and phloem removed to prevent the interference of water sources. Samples were frozen and stored in the lab until cryogenic vacuum extraction (as per Koeniger et al. (2011) using 60-90min extraction time per sample). Extracted water was measured using CRDS (Picarro L2130-i).

Insitu Sampling

Collected soil and xylem vapour samples were attached to bottles filled with desiccant (Drierite W. A. Hammond DRIERITE Co. LTD, Xenia, OH, USA) to dry incoming air to the laser spectrometer (Picarro L2130-i). Vapour sampling of each soil or xylem location was conducted for 10 min periods to establish stable vapour concentration (plateaus) to the laser spectrometer. Measurement for each location was conducted at 2-hour intervals.

Text S2: Energy Balance and EcH2O development

Plant hydraulics are resolved using the Soil Plant Atmosphere Continuum module (SPAC) which tracks leaf water potential and conductivity limitations due to cavitation (Simeone et al., 2019). The SPAC module includes supply-demand functions in the rhizosphere (as a function of soil hydraulic conductivity, root area index, and pore-disconnectedness index), and stem and leaf (function of vegetation conductivity and leaf area index). The supply-demand further regulates transpiration by soil and vapour pressure deficits. Initial testing of the study site using the SPAC module did not reveal sensitivity due to high continued water use of the willows during the growing season and was therefore deactivated prior to calibration.

Table S1: Calibrated soil parameters for below Willow and Grass, presented as the mean, standard deviation (±), and skew. Note: field capacity is not directly calibration, but is a function of Brooks-Corey, air entry pressure, porosity, and residual moisture content. SPAC module was evaluated prior to calibration (insensitive) and was deactivated for calibration (parameters not shown).

	Willow		**Grass**	
	Soil Parameters			
	Mean ± std	**Skew**	**Mean (std)**	**Skew**
Albedo	0.25 ± 0.11	-0.01	0.22 ± 0.06	-0.39
Brooks-Corey Lambda	3.76 ± 0.68	0.46	3.78 ± 0.92	-0.09
Air entry pressure [m]	0.24 ± 0.12	0.56	0.14 ± 0.12	0.96
Field Capacity	0.2 ± 0.01	-0.09	0.16 ± 0.01	0.02
Porosity [m^3/m^3]	0.41 ± 0.02	-0.06	0.4 ± 0.02	-0.39
Residual Moisture Content [m^3/m^3]	0.01 ± 0.01	0.11	0.01 ± 0	0.03
Vertical Conductivity [m/s]	1.1E-4 ± 9E-5	1.01	6.8E-4 ± 2E-4	0.24
	Vegetation Parameters			
	Mean ± std	**Skew**	**Mean (std)**	**Skew**
Root Aspect Ratio (horizontal)	2.73 ± 0.47	0.93	0.57 ± 0.28	-0.2
Canopy Water Storage [m/LAI]	0.74E3 ± 0.14E3	1.23	1.39E3 ± 0.3E3	0.42
Maximum stomatal conducance [m/s]	0.49E-2 ± 0.13E-2	2.35	1.64E-2 ± 0.61E-2	1.39
Stomatal conducance light coefficient	512.44 ± 121.87	1.34	323.3 ± 119.96	-0.39
Stomatal conducance VPD coefficient [Pa]	1.35E4 ± 1.29E4	0.79	0.23E4 ± 0.25E4	1.26
Root Distribution Parameter (K_{root})	13.33 ± 3.98	0.79	8.21 ± 1.05	0.35
Maximum LWP for stomatal conductance	0.11 ± 0.12	1.57	0.48 ± 0.3	0.08
Wilting Point [m^3/m^3]	0.04 ± 0.01	0.59	0.04 ± 0.01	-0.08
	Vegetation Biomass Parameters			
	Mean ± std	**Skew**	**Mean (std)**	**Skew**
Vegetation Water Use Parameter 1	0.82 ± 0.11	-0.10	0.76 ± 0.10	0.74
Vegetation Water Use Parameter 2	4.17 ± 2.76	0.25	5.23 ± 2.52	-0.07
Water Use Efficiency [gCm^{-1}]	1.6E4 ±1.2E4	1.25	2.54E3 ± 7.99E3	4.59

Foliage allocation coefficient a [m^2KgC^{-1}]	0.06 ± 0.06	1.04	N/A	N/A
Foliage allocation coefficient b [m^2KgC^{-1}]	0.91 ± 0.02	1.17	N/A	N/A
Stem allocation coefficient a	0.25 ± 0.33	1.81	N/A	N/A
Minimum tree height to stem ratio	5.07 ± 3.01	-0.08	N/A	N/A
Wood Density [gCm^{-2}]	6.36E4 ± 3.39E4	0.31	N/A	N/A
Specific Leaf Area [m^2KgC^{-1}]	2.74 ± 0.76	-0.30	3.06 ± 0.93	-1.20
Leaf Turnover [s^{-1}]	5.27E-8 ± 2.65E-8	0.73	5.16E-7 ± 5.00E-8	-0.23
Maximum Leaf Turnover Due To Water Stress [s^{-1}]	5.65E-7 ± 1.58E-7	0.62	N/A	N/A
Water Stress Parameter	5.31 ± 2.87	-0.22	N/A	N/A
Maximum Leaf Turnover Due To Temperature Stress [s^{-1}]	5.68E-7 ± 5.73E-7	1.29	N/A	N/A
Temperature Stress Parameter	6.61 ± 3.47	0.35	N/A	N/A
Dry Leaf Turnover Rate [s^{-1}]	N/A	N/A	1.01E-6 ± 2.94E-7	1.22
Dry Leaf Turnover Adjustment Parameter	N/A	N/A	5.25 ± 2.72	1.12

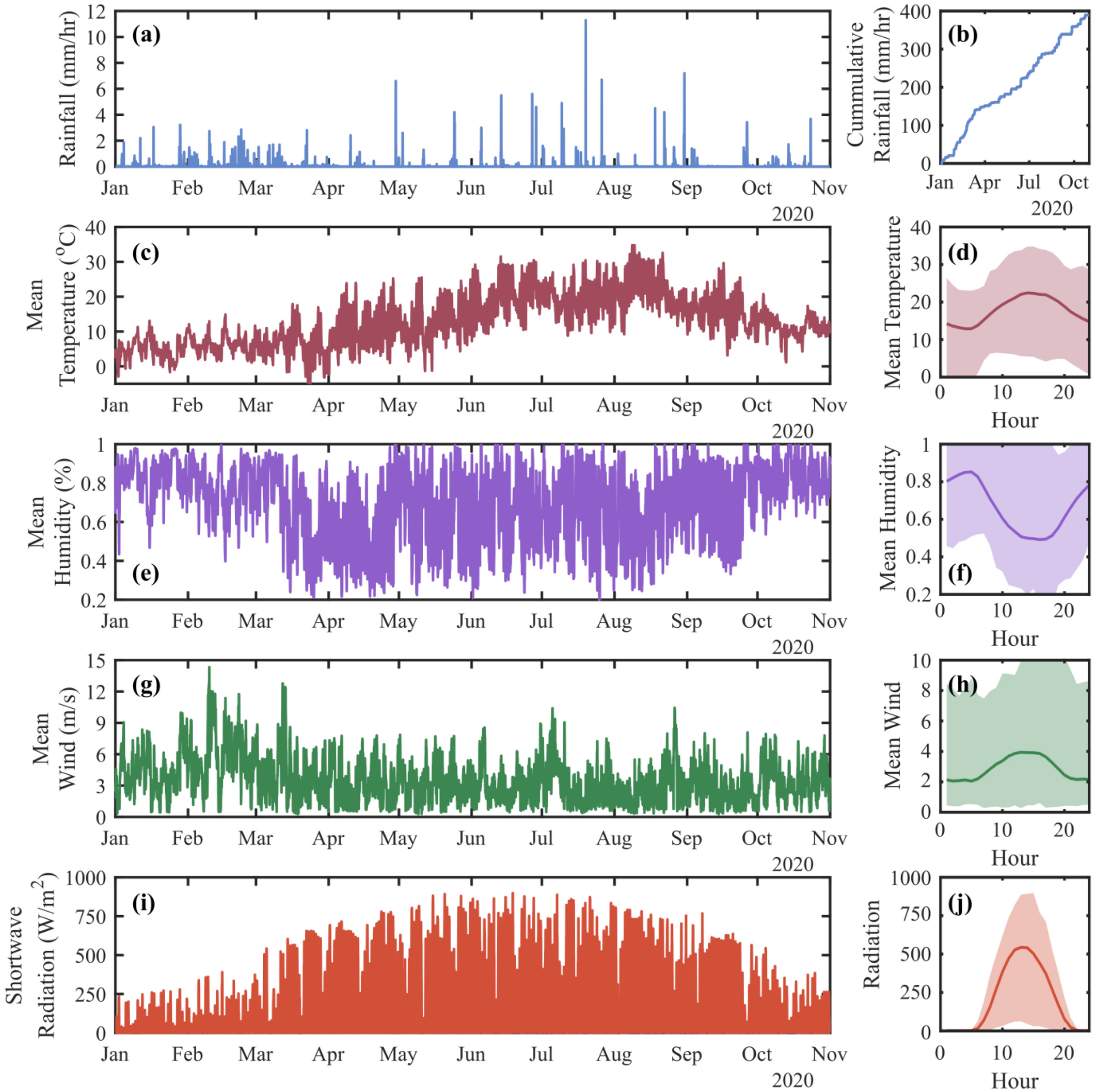


Figure S2: Climate data used within EcH$_2$O-iso for the study site between January and November 2020. (a) Hourly precipitation, (b) cumulative precipitation, (c) mean hourly temperature, (d) mean diel temperature (and range) during the growing season (May –September), (e) mean hourly relative humidity, (f) mean diel humidity (and range) during the growing season (May –September), (g) mean hourly wind speed, (h) mean diel wind speed (and range) during the growing season (May –September), (i) mean hourly shortwave radiation, and (j) mean diel radiation (and range) during the growing season (May –September).

Table S2: Average and standard deviation of the goodness-of-fit criteria for modelled time-series of soil, vegetation, and energy balance datasets. *Dataset was not used in calibration. **Isotope measurement uncertainty shows the average range of sub-daily variability (average measurement uncertainty in parentheses) – for processes not included in EcH2O-iso – and uncertainty of the LMWL regression (lc-excess). ^{H}Sub-discretized soil moisture at 10cm.

			Site A		**Site B**	
			MAE	Measurement Uncertainty**	MAE	Measurement Uncertainty**
Soil	Layer 1 (0-10cm)	VMC [m3/m3]	0.03 ± 0^{H}	0.025	0.02 ± 0	0.025
		δ^2H [‰]	8.6 ± 0.1	11.9 (0.7)	5.7 ± 0.2	2 (0.7)
		lc-excess [‰]*	9.3 ± 0.7	9	4.5 ± 0	6.9
	Layer 2 (10-40cm)	VMC [m^3/m^3]	0.02 ± 0	0.025	0.04 ± 0.01	0.025
		δ^2H [‰]	4.2 ± 1.4	1.3 (0.7)	2.4 ± 0.4	1.74 (0.7)
		lc-excess [‰]	2.8 ± 0.3	5.6	2.1 ± 0	6.1
	Layer 3 (40-100cm)	VMC [m^3/m^3]	0.06 ± 0.05	0.025	0.01 ± 0.01	0.025
		δ^2H [‰]	6.8 ± 1.5	0.8 (0.7)	1.3 ± 0.1	1.6 (0.7)
		lc-excess [‰]	1.8 ± 0	5.7	4.6 ± 0.1	6
Vegetation	Flux	Sapflow [m^3/s]	0.023 ± 0.003	0.016	NA	NA
	Biomass	LAI (Willow 1) [m^2/m^2]	0.5 ± 0.2	0.9	NA	NA
		LAI (Willow 2) [m^2/m^2]	0.5 ± 0.2	0.9	NA	NA
		LAI (Grass) [m^2/m^2]	NA	NA	0.1 ± 0	NA
		Basal Area (Willow 1) [µm]	1.5 ± 0.7	0.6	NA	NA
		Basal Area (Willow 2) [µm]	2.2 ± 1	0.6	NA	NA
Energy Balance	Soil Temperature*	10 cm [^{o}C]	2 ± 0.3	0.4	1.2 ± 0.1	0.3
		40 cm [^{o}C]	2.4 ± 0.5	0.2	1.9 ± 0.2	0.2
		100 cm [^{o}C]	1.4 ± 0.5	0.2	2.8 ± 0.2	0.2
	Surface Temperature [^{o}C]		NA	NA	1.8 ± 0.2	0.6
	Latent Heat [W/m^2]		NA	NA	20.5 ± 0.7	13.9
	Sensible Heat [W/m^2]		NA	NA	4.5 ± 0.2	7.1

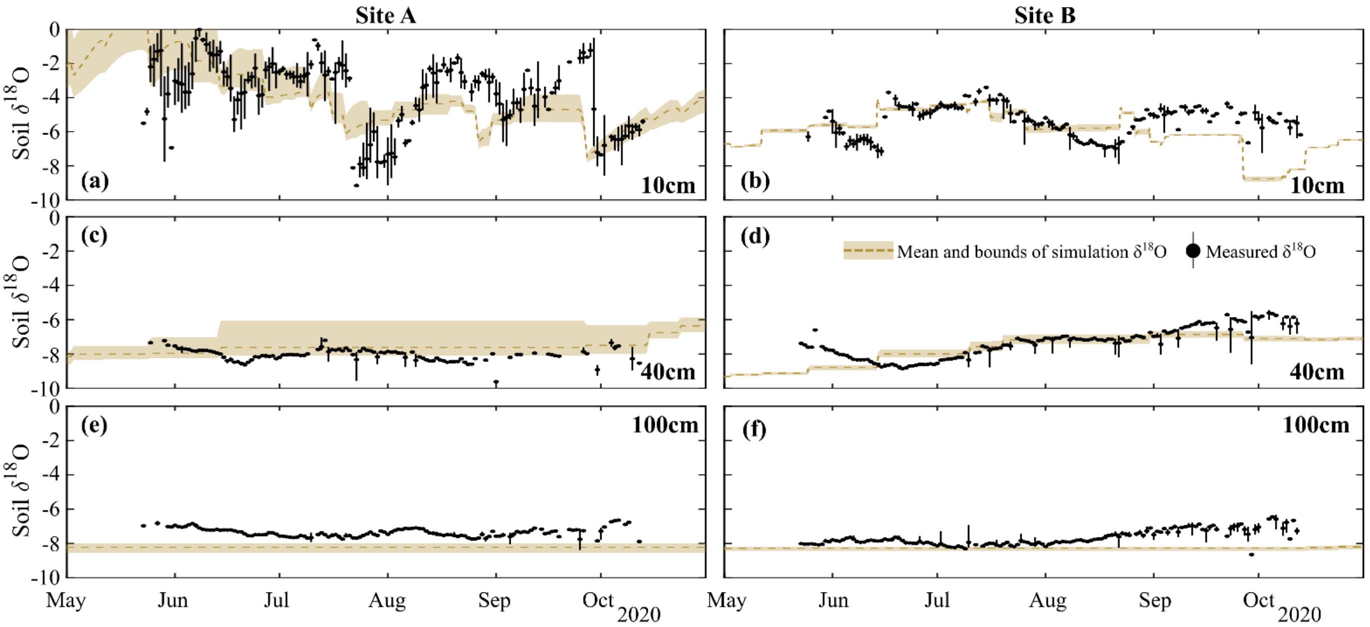
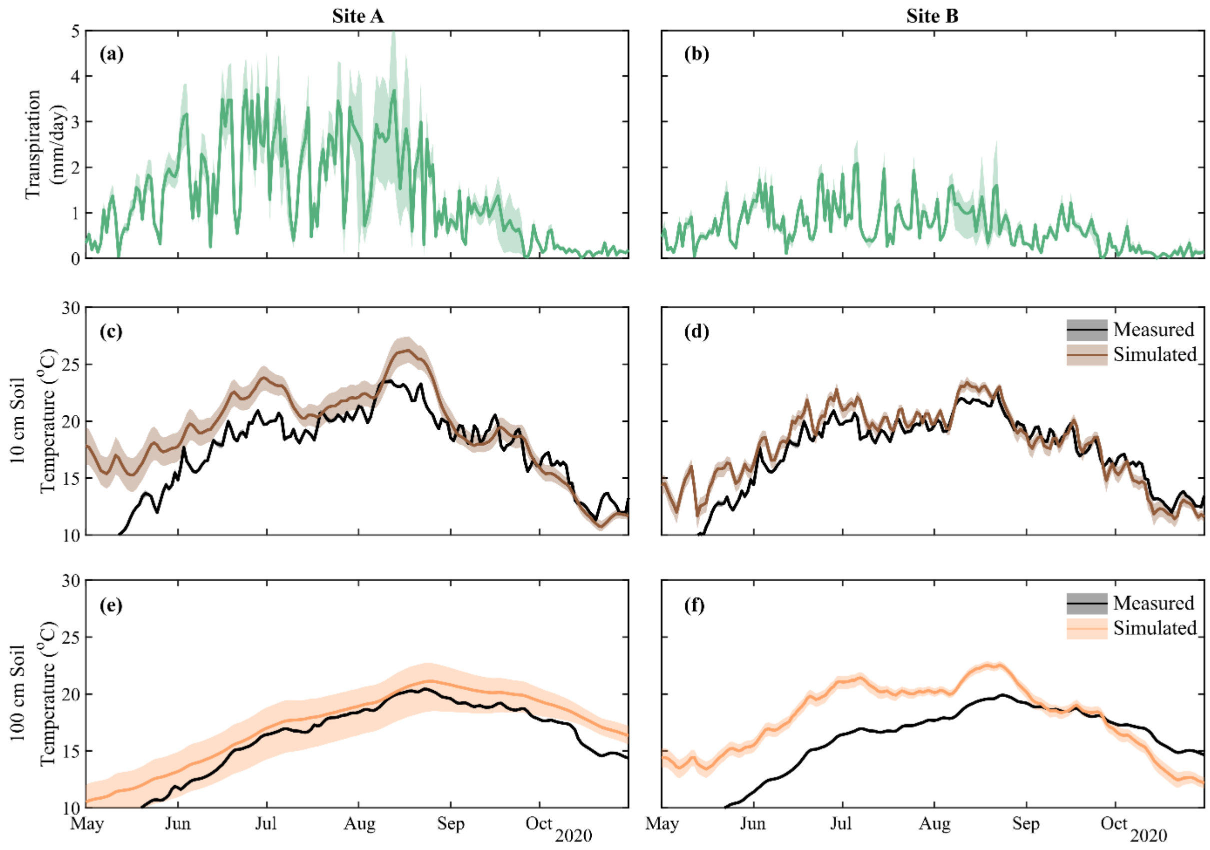


Figure S3: Measured and simulated soil δ18O at Site A and B at 10cm (a and b), 40cm (c and d), and 100cm (e and f).



55 **Figure S4: Simulated transpiration rate (mm/day) for (a) Site A (Willow only) and (b) Site B (Grass). Simulated and measured soil temperature at 10cm at (c) Site A, and (d) Site B, and at 100cm at (e) Site A, and (f) Site B.**

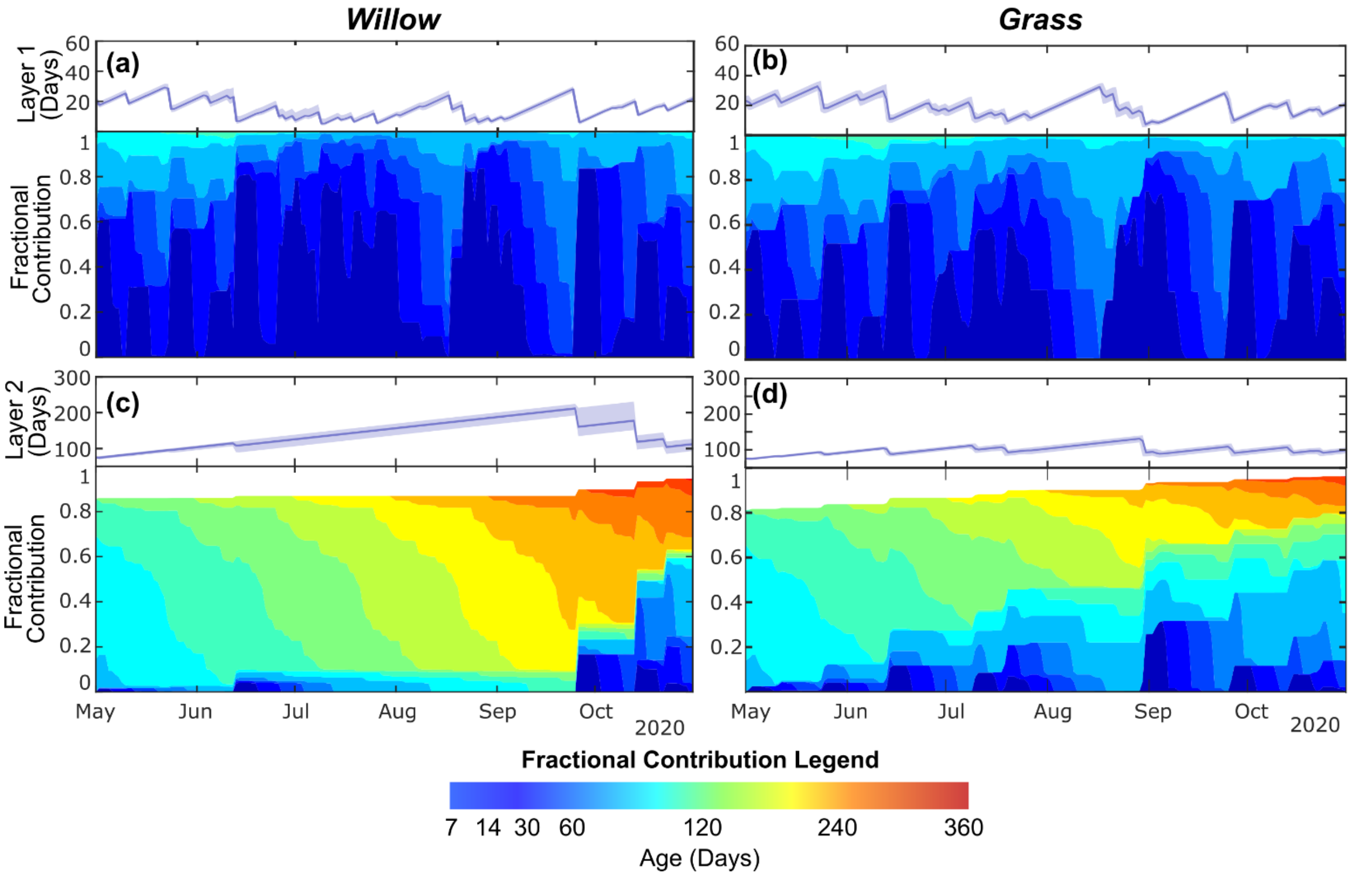


Figure S5: Cumulative proportion of water in storage and in root-uptake from each month since the beginning of the simulation (January). White regions indicate water is older than the simulation

Table S3: Proportion of water in storage or flux for the willows older than or equal to precipitation in each month (e.g. older than or equal to January precipitation). Proportions are displayed for each period of the growing season. N/A indicates not applicable.

	Willow								
	May 1 - June15			*June 15-July31*			*Aug1 - Oct31*		
	Layer 1	*Layer 2*	*RWU*	*Layer 1*	*Layer 2*	*RWU*	*Layer 1*	*Layer 2*	*RWU*
≥ *Jan*	0.00	0.27	0.07	0.00	0.25	0.05	0.00	0.21	0.05
≥ *Feb*	0.02	0.80	0.21	0.00	0.75	0.13	0.00	0.64	0.08
≥ *Mar*	0.13	0.97	0.33	0.00	0.91	0.16	0.00	0.77	0.09
≥ *Apr*	0.42	0.99	0.56	0.01	0.93	0.17	0.00	0.79	0.09
≥ *May*	0.89	1.00	0.91	0.04	0.95	0.20	0.00	0.81	0.09

≥ *June*	1.00	1.00	1.00	0.46	1.00	0.53	0.00	0.85	0.09
≥ *July*	N/A	N/A	N/A	1.00	1.00	1.00	0.19	0.85	0.24
≥ *Aug*	N/A	N/A	N/A	N/A	N/A	N/A	0.55	0.87	0.57
≥ *Sept*	N/A	N/A	N/A	N/A	N/A	N/A	0.86	0.96	0.87
≥ *Oct*	N/A	N/A	N/A	N/A	N/A	N/A	1.00	1.00	1.00

Table S4: Proportion of water in storage or flux for the grass older than or equal to precipitation in each month (e.g. older than or equal to January precipitation). Proportions are displayed for each period of the growing season. N/A indicates not applicable.

	Grass								
	May 1 - June15			*June 15-July31*			*Aug1 - Oct31*		
	Layer 1	*Layer 2*	*RWU*	*Layer 1*	*Layer 2*	*RWU*	*Layer 1*	*Layer 2*	*RWU*
≥ *Jan*	0.00	0.29	0.19	0.00	0.21	0.14	0.00	0.12	0.11
≥ *Feb*	0.03	0.76	0.42	0.00	0.54	0.29	0.00	0.30	0.20
≥ *Mar*	0.18	0.92	0.57	0.01	0.66	0.35	0.00	0.37	0.24
≥ *Apr*	0.48	0.95	0.73	0.03	0.71	0.38	0.00	0.39	0.25
≥ *May*	0.93	0.99	0.96	0.11	0.80	0.46	0.00	0.45	0.28
≥ *June*	1.00	1.00	1.00	0.59	0.94	0.75	0.03	0.56	0.33
≥ *July*	N/A	N/A	N/A	1.00	1.00	1.00	0.28	0.72	0.50
≥ *Aug*	N/A	N/A	N/A	N/A	N/A	N/A	0.59	0.91	0.75
≥ *Sept*	N/A	N/A	N/A	N/A	N/A	N/A	0.86	0.98	0.92
≥ *Oct*	N/A	N/A	N/A	N/A	N/A	N/A	1.00	1.00	1.00

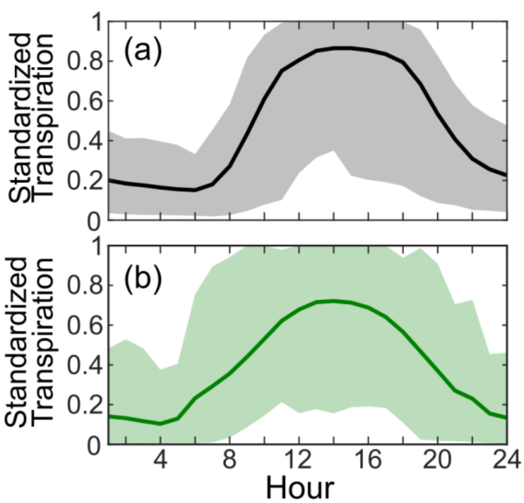


Figure S6: Hourly variability of standardized (0 to maximum transpiration) of (a) measured sap flow, and (b) simulated transpiration.

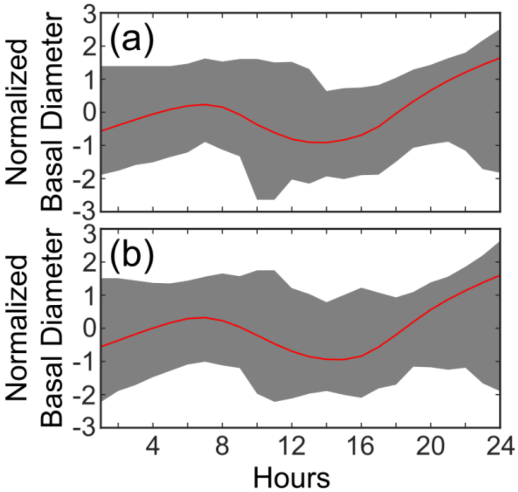


Figure S7: Normalized daily basal diameter for (a) Willow 1 and (b) Willow 2

Table S5: Average (± standard deviation) transit time in hours of root water in each layer to 1m measurement height in Willow 1 and Willow 2 and the average (± standard deviation) of root length for each soil layer

	Transit Time				**Root Length (m)**
	Simulated Data		**Measured Data**		
Soil Layer	**Willow 1 (hr)**	**Willow 2 (hr)**	**Willow 1 (hr)**	**Willow 2 (hr)**	
Layer 1	160.0 ± 21.2	140.5 ± 3.8	217.3 ± 40.0	196.0 ± 44.8	4.0 ± 0.5
Layer 2	205.0 + 97.3	82.1 ± 12.1	224.0 ± 127.4	160.7 ± 23.5	1.6 ± 0.5
Layer 3	85.2 ± 26.8	78.8 ± 8.4	85.6 ± 1.0	132.8 ± 10.3	0.5 ± 0.2

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