Table S1: Calibrated parameters of the EcoHydroPlot.

Module	Parameter	Description	Unit
Water flux	**rE**	Radiation extinction factor as a function of sun angle, the distribution of plants, and the arrangement of leave	
	alpha	Interception threshold parameter	mm
	Ic	Maximum infiltration capacity	
	ks1	Saturated hydraulic conductivity @ Shallow soil layer	mm d^{-1}
	ks2	Saturated hydraulic conductivity @ Deep soil layer	mm d^{-1}
	Smax	Maximum soil moisture content @ Shallow soil layer	mm
	GWmax	Maximum soil moisture content @ Deep soil layer	mm
	g1	Nonlinear scaling parameter @ Shallow soil layer	
	g2	Nonlinear scaling parameter @ Deep soil layer	
	PF_Scale	Preferential flow path parameter	
Deuterium	**INTp**	Passive storage mixing volume @ Tree canopy	mm
	stoSp	Passive storage mixing volume @ Shallow soil layer	mm
	gwSp	Passive storage mixing volume @ Deep soil layer	mm
	k	Seasonality factor	
	x	Water vapour mixing ratio	

Table S2: Selected governing equations of EcoHydroPlot for the two-layer configuration used in this study, modified from Landgraf et al (2023). For details, please refer to the original paper (Landgraf et al., 2023).

Process	Equation
1. Craig–Gordon fractionation and surface cover	
Equilibrium fractionation (α_e)	$\alpha_e = exp[\frac{1}{1000} \times (\frac{1158.8 \cdot T_k{}^3}{10^9} - \frac{1620.1 \cdot T_k{}^2}{10^6} + \frac{794.84 \cdot T_k}{10^3} - 161.04 + \frac{2.9992 \cdot 10^9}{T_k{}^3})]$
Equilibrium separation (ε_e)	$\varepsilon_e = (\alpha_e - 1) \cdot 1000$
Kinetic fractionation (ε_k)	$\varepsilon_k = n(1 - n) \cdot 1000 \cdot (1 - RH), n = 0.9755$
Atmospheric vapour composition (δ_A)	$\delta_A = \frac{-58.7 - k \cdot \varepsilon_e}{1 + k \cdot \varepsilon_e \cdot 10^{-3}}$
Limiting isotopic composition (δ*)	$\delta * = \frac{RH \cdot \delta_A + \varepsilon_k + \frac{\varepsilon_e}{\alpha_e}}{RH - 10^{-3}\left(\varepsilon_k + \frac{\varepsilon_e}{\alpha_e}\right)}$
Enrichment slope (m)	$m = \frac{RH - 10^{-3}\left(\varepsilon_k + \frac{\varepsilon_e}{\alpha_e}\right)}{1 - RH + 10^{-3} \cdot \varepsilon_k}$
2. Separation of potential ET	
Surface cover fraction (SCF)	$SCF = 1 - exp(r_E \cdot LAI)$
Potential transpiration (T_p)	$T_p = PET \cdot SCF$
Potential soil evaporation (E_p)	$E_p = PET \cdot (1 - SCF)$
3. Water flux at interception	
Interception capacity (I_max)	$I_{max} = \alpha \cdot LAI$
Available interception store (I_avail)	$I_{avail} = I_{max} - I$
Canopy drainage (D)	$D = I_{avail} \cdot \left(1 - \frac{1}{1 + \frac{SCF \cdot P}{I_{avail}}}\right)$
Interception evaporation (E_i)	$E_i = min(E_p, I)$
4.* Water flux at *shallow soil water storage	
Preferential flow (Pref_Flow)	$if\ P_N > 4.2\ mm\ d^{-1}, Pref_{Flow} = P_N \cdot PF_{Scale}$
Transpiration, upper (Tr_Upper)	$Tr_{Upper} = \frac{STO}{S_{max}} \cdot T_p$
Soil evaporation (E_s)	$E_s = \frac{STO}{S_{max}} \cdot E_p$
Percolation (Perc)	$if\ P_N > 0, Perc = k_{s1} \cdot \left(\frac{STO}{S_{max}}\right)^{g_1}$
Shallow soil water storage (STO)	$STO^{(t)} = STO^{(t-1)} + P_N - Tr_{Upper} - E_s - Perc$
5.* Water flux at d*eep soil water storage	
Transpiration, lower (Tr_Lower)	$Tr_{Lower} = \frac{GW}{GW_{max}} \cdot T_p$
Groundwater flow (GW_flow)	$if\ Perc > 0, GW_{flow} = k_{s2} \cdot \left(\frac{GW}{GW_{max}}\right)^{g_2}$
Deep soil water storage (GW)	$GW^{(t)} = GW^{(t-1)} + Perc + Pref_{Flow} - Tr_{Lower} - GW_{flow}$
5. δ^2H tracking in interception	
Interception mixing volume (Int_D)	$Int_D = I - D + E_i + T_h + INTp$

Interception δ²H (Int_CD)	$Int_{CD}{}^{(t)} = \frac{Int_D \cdot Int_{CD}{}^{(t-1)} + D \cdot \delta_P}{Int_D + D}$
Rayleigh-enriched interception (Idl_H)	$Idl_H = (Int_{CD} - \delta *) \cdot (1 - x)^m + \delta *$
Flux δ²H from interception (fInt_CD)	$fInt_{CD} = \frac{Int_D \cdot Int_{CD} - E_i \cdot Idl_H}{Int_D}$
Interception evap. vapour (IdE_H)	$IdE_H = \frac{\frac{Idl_H - \varepsilon_e}{\alpha_e} - RH \cdot \delta_A - \varepsilon_k}{1 - RH + 10^{-3} \cdot \varepsilon_k}$
6. δ^2H tracking in *shallow soil water storage*	
Upper mixing volume (upSTO_D)	$upSTO_D = STO - P_N - T_h + E_s + Tr_{Upper} + Perc + stoSp$
Upper storage δ²H (upCSTO_D)	$upCSTO_D{}^{(t)} = \frac{upSTO_D \cdot upCSTO_D{}^{(t-1)} + T_h \cdot fInt_{CD} + P_N \cdot \delta_P}{upSTO_D + P_N + T_h}$
Rayleigh-enriched upper store (Sdl_H)	$Sdl_H = (upCSTO_D - \delta *) \cdot (1 - x)^m + \delta *$
Flux δ²H from upper store (fupCSTO_D)	$fupCSTO_D = \frac{upSTO_D \cdot upCSTO_D - E_s \cdot Sdl_H}{upSTO_D - E_s}$
Soil evap. vapour (SdE_H)	$SdE_H = \frac{\frac{Sdl_H - \varepsilon_e}{\alpha_e} - RH \cdot \delta_A - \varepsilon_k}{1 - RH + 10^{-3} \cdot \varepsilon_k}$
7. δ^2H tracking in *deep soil water storage*	
Lower mixing volume (gwSTO_D)	$gwSTO_D = GW - Perc - Pref_{Flow} + GW_{flow} + Tr_{Lower} + gwSp$
Lower storage δ²H (gwCSTO_D)	$gwCSTO_D{}^{(t)} = \frac{gwSTO_D \cdot gwCSTO_D{}^{(t-1)} + Perc \cdot fupCSTO_D + Pref_{Flow} \cdot \delta_P}{gwSTO_D + Perc + Pref_{Flow}}$
8. δ^2H tracking in *deep soil water storage*	
Transpiration / xylem δ²H (Tr_D)	$Tr_D = \frac{Tr_{Upper} \cdot fupCSTO_D + Tr_{Lower} \cdot gwCSTO_D}{Tr_{Upper} + Tr_{Lower}}$

T_k = air temperature in K, AT + 273.15

I = interception storage

T_h = throughfall

n = diffusivity ratio

Parameters as in Table S1

Table S3: Calibration ranges and calibrated values (median and range across the 100 behavioural parameter sets) of the EcoHydroPlot parameters.

Parameter	Calibration range	Calibrated (median)	Behavioural range
rE	-0.5 - -0.1	-0.253	-0.463 - -0.212
alpha	0.1 - 4.0	0.403	0.107 - 0.464
Ic	40 - 80	69.59	49.48 - 77.17
ks1	0.1 - 10.0	7.51	0.58 - 8.38
ks2	0.1 - 10.0	9.34	6.13 - 9.98
Smax	30 - 100	83.30	78.94 - 86.25
GWmax	100 - 600	598.80	590.40 - 599.64
g1	1.0 - 3.0	2.90	1.35 - 3.00
g2	2.0 - 5.0	2.02	2.00 - 2.08
PF_Scale	0.1 - 0.9	0.336	0.306 - 0.369
INTp	0.5 - 2.0	0.706	0.504 - 1.969
stoSp	1.0 - 20.0	1.195	1.012 - 3.490
gwSp	5.0 - 150.0	16.15	7.78 - 49.65
k	0.3 - 0.9	0.880	0.776 - 0.898
x	0.3 - 0.9	0.324	0.305 - 0.418

Note: Ranges were adapted from a previous application at the Demnitzer Millcreek Catchment (Landgraf et al., 2023), and most of ranges were widened.

Several parameters converged close to a limit. Those on ks2 (to upper limit), g2 (to lower limit) and GWmax (to upper limit, already widened from 50-90 to 100-600 mm) were retained because wider values gave groundwater recharge that was physically implausible for the observed dry soil.

stoSp and k have been converged to physically plausible limit. stoSp converged on the smallest plausible passive mixing volume. k is bounded by definition ($0 < k < 1$) and expected at 0.5-0.8 in temperate regions. Its limit was raised to 0.9 for the summer study period but no further, as the site is not tropical.

Calibration range of x is set to the referential range from Landgraf et al. (2023) with widened upper limit. A diagnostic re-calibration with the prior on x opened to 0.05-0.95 moved its behavioural range to 0.052-0.104, confirming that the original lower limit truncated the posterior. The mean KGE, however, changed by only +0.002 (0.5315 to 0.5338), and the simulated time series differed by less than 4% of the observed range for every target, because the other parameters compensated (e.g. alpha shifted from 0.13 to 3.83, k from 0.88 to 0.45). The parameter values are therefore strongly compensating, whereas the structural signature of the error, which this study analyses, is unaffected.

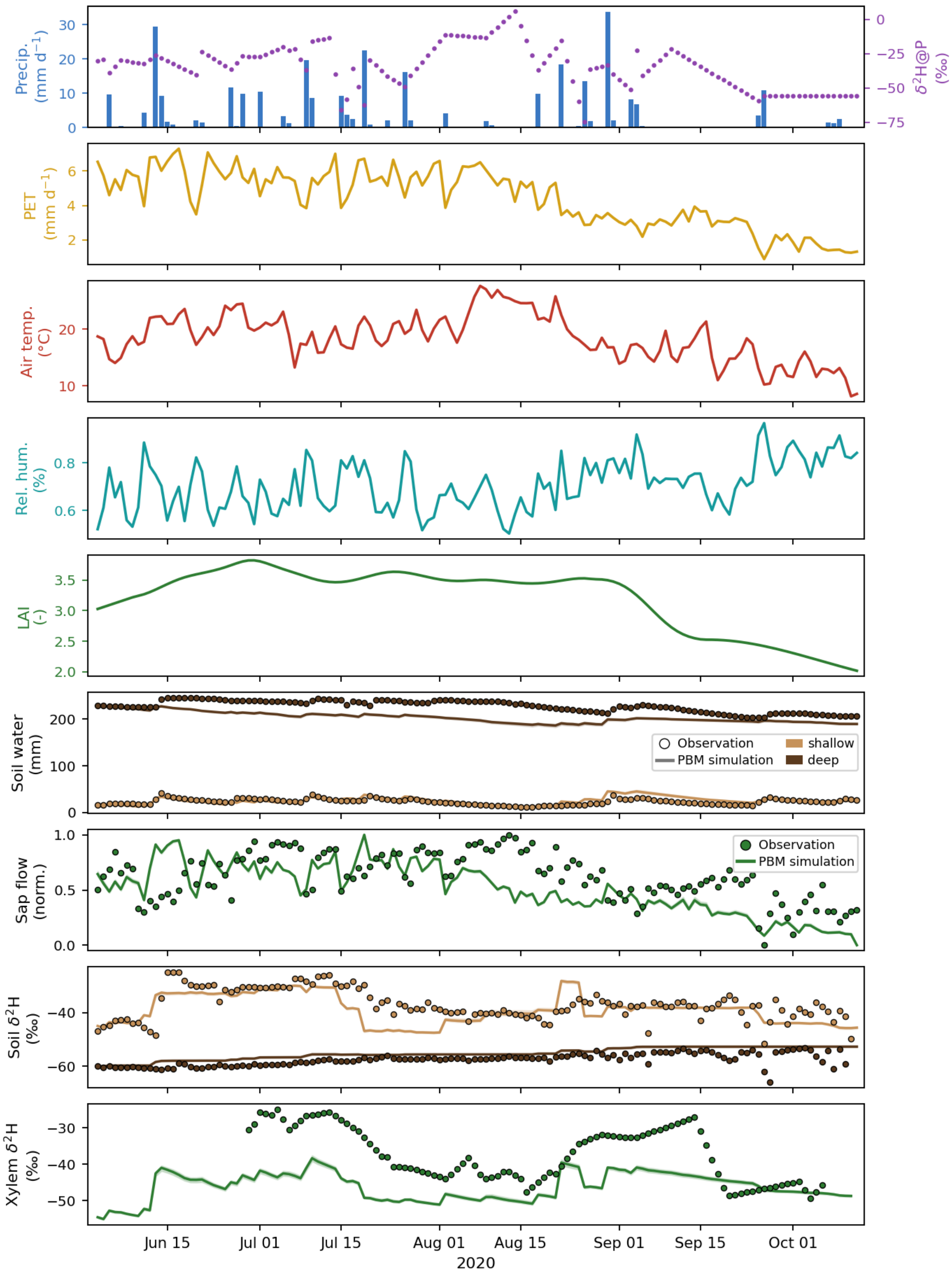

Figure S1: Model forcing (precipitation and precipitation δ²H, PET, air temperature, relative humidity, LAI) and model performance. Observations (points) were compared with EcoHydroPlot simulation (lines) for all 6 targets. EcoHydroPlot simulation ranges across the behavioural parameters for shown in shade.

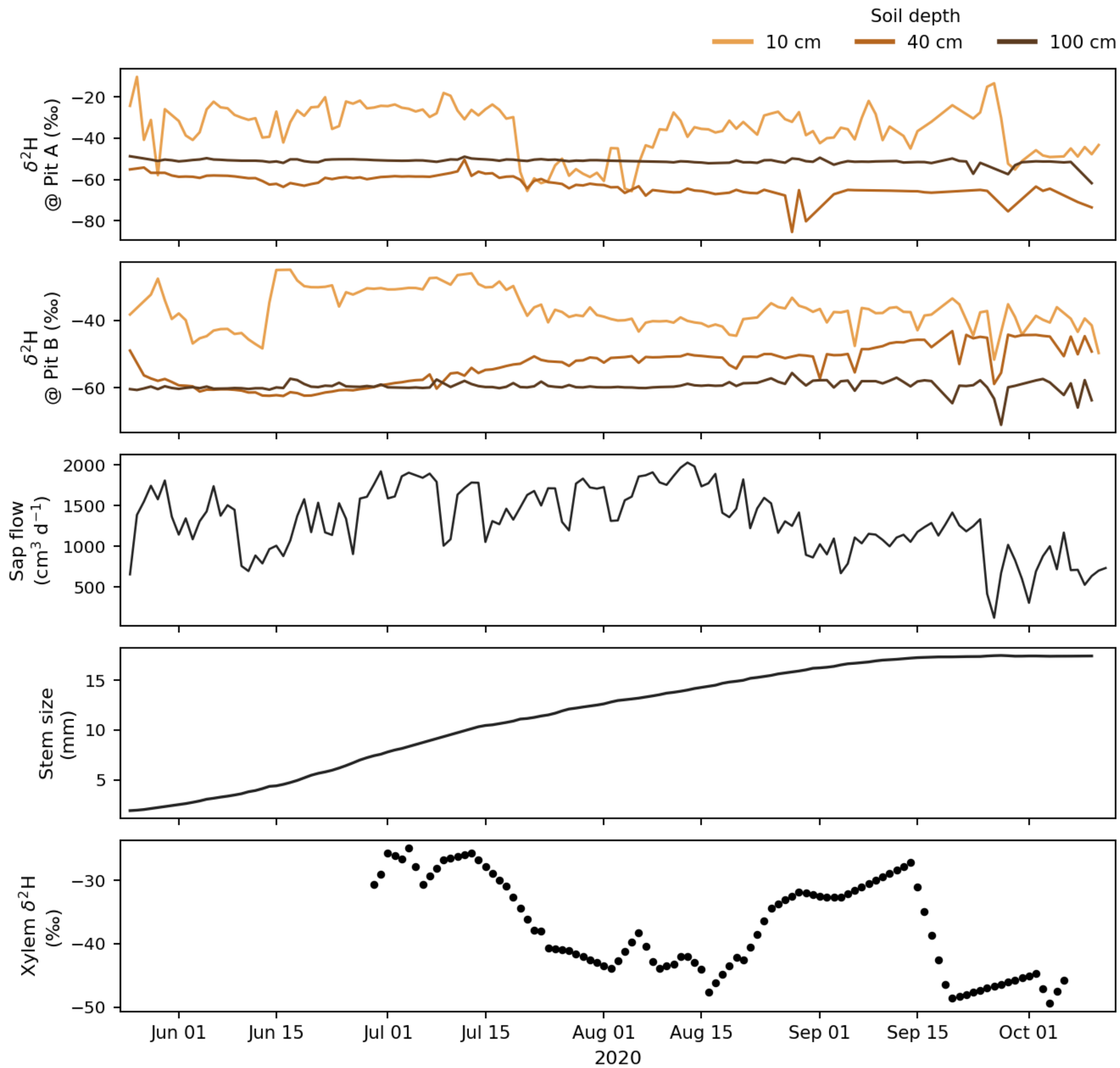

Figure S2: Soil δ²H at Pit A and Pit B (10, 40, 100 cm), sap flow, stem size, and xylem δ²H were monitored at the willow plot over 2020. For model run, Pit A and Pit B were averaged at each depth.

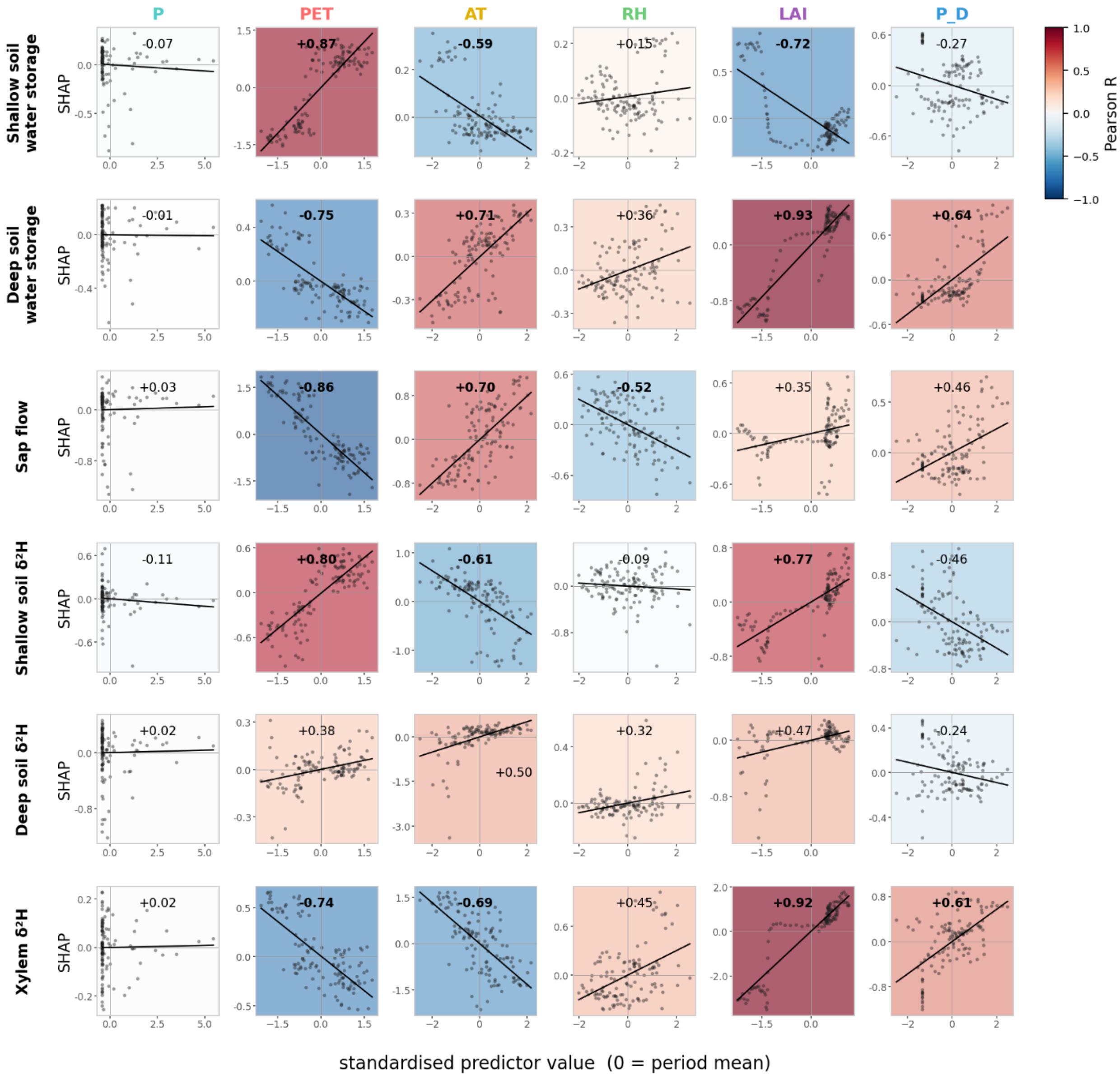

Figure S3: Correlation relationship between each predictor's SHAP contribution to the PBM error and the standardised predictor value (0 = study period mean), for the six targets (rows) and six predictors (columns: Precipitation, PET, Atmospheric Temp., Relative Humidity, LAI, δ²H at precipitation). Background shading and inset value show the Pearson R value.