Supplementary materials:

Appendix A: Hydrological components in the original STARR model

The main reservoir structures in the model consist of four parts: canopy interception, soil storage, stream water, and groundwater storage, while the dynamics and interactions of these storages are determined by the hydrological processes (e.g., Rainfall, Evapotranspiration (ET), Infiltration, Seepage, Capillary flux and etc.) (Fig. 1). All equations are summarised in Table S1. Interception is replenished through a certain fraction of the rain hitting the canopy and the flux processes (throughfall) are simulated following Rutter et al. (1972), while the maximum interception storage capacity depends on the leaf area index (LAI; Von Hoyningen-Huene, 1981). Potential evapotranspiration (PET) is calculated following the method in the HYPE (Hydrological Predictions for the Environment) model (Lindström et al., 2010), while the actual evapotranspiration is subject to water availability in interception and soil storage. Instantaneous surface runoff is produced when soil storage exceeds the maximum storage capacity, while the discharge from soil and groundwater to the stream is linearly related to soil and groundwater storage, respectively. These three runoff components constitute streamflow and flow routing of all runoff components is determined by setting a fixed celerity. The soil and groundwater storages are interconnected through seepage (from soil to groundwater) and capillary flux (from groundwater to soil), both of which depend on the soil storage value in relation to maximum soil storage capacity. Lateral groundwater flow processes are linearly determined by the slope of the landscape.

Isotope signatures of each water component are calculated through mass balance equations, assuming the mixing is complete and instantaneous. Isotope fractionation is only considered in the interception storage and conceptualized as an empirical relationship on the basis of a simple linear regression of deuterium signatures in gross rain. The ratio of the transpiration in ET is determined by $(\delta_A-\delta_E)/(\delta_S-\delta_E)$ assuming that transpiration is a non-fractionation process

(Chakraborty et al., 2018), where δ_A, δ_E, δ_S are the isotopic compositions of ambient atmospheric vapour, evaporation and soil water, respectively (Correa et al., 2020).

Table S1. The modified STARR model components and equations.

Process	Equations	Variables
	Interception storage (Stevenson et al., 2023)	
Interception per timestep	$INV = (\alpha \times LAI) \times (1 - \frac{1}{1 + \frac{SCF \times P}{\alpha \times LAI}})$	α: Empirical parameter LAI: Leaf area index SCF: Surface Cover Fraction P: Rainfall
Surface Cover Fraction	$SCF = 1 - e^{rE \times LAI}$	rE: Radiation extinction
Maximum interception capacity	$C_{sat} = 0.2001 + LAI \times 0.3001$	C_{sat}: canopy saturation volume
Evaporation from interception	*If* $INT < E_p$: $E_i = INT$ *Else:* $E_i = E_p$	INT: interception storage
Drainage (Rutter et al., 1972)	*If* $INT > C_{sat}$: $D = D_s \times e^{b \times (INT - C_{sat})}$ *Else:* $D = 0$	INT: Interception storage D: Drainage volume D_s: Empirical parameter b: Empirical parameter
	Transpiration (Stevenson et al., 2023)	
Potential transpiration Potential evaporation	$T_p = PET \times SCF$ $E_p = PET - T_p$	
	Soil storage	
Instantaneous surface runoff	$Q_s = \max(STO - FC, 0)$	STO: Soil water storage FC: Soil water storage capacity
Evaporation from soil	If $STO < LP \times FC$: $E_s = \frac{E_p - E_i}{LP \times FC}$ Else: $E_s = E_p - E_i$	LP: Fraction of soil water capacity above which $E_s = E_p$
Transpiration from soil	$T_s = T_p \times \frac{STO}{FC}$	
Seepage	$Seepage = \frac{STO}{FC^{\beta}}$	β: Empirical parameter
Soil discharge	$Q_{STO} = STO \times k_s$	k_s: Empirical parameter
	Groundwater storage	
Capillary flux	$CapFlux = C_{flux} \times \frac{FC - STO}{FC}$	C_{flux}: maximum capillary rise
Transpiration from groundwater	$T_g = (T_p - T_s) \times \frac{STO}{GW_{max}}$	GW_{max}: maximum groundwater storage
Groundwater discharge	$Q_{GW} = GW \times k_g$	k_g: Empirical parameter GW: Groundwater storage

Lateral flow	$Q_{lf} = k_{sat} \times slope(\frac{DEM}{1000} + GW)$	k_{sat}: horizontal saturated conductivity $slope$: slope gradient

Table S2. Initial ranges of the STARR model parameters.

Parameter	Unit	Description	Initial range
		Interception storage	
$\boldsymbol{\alpha}$	[cm/day]	Interception threshold parameter	0.5 - 3.5
$\boldsymbol{rE}$	[-]	Radiation extinction by the canopy	0.2 - 0.8
$\boldsymbol{D_s}$	[mm/day]	Drainage from canopy when the storage is full	0.1 - 1.2
$\boldsymbol{b}$	[-]	Exponent in Rutter interception module	0.1 - 1.2
		Soil Storage	
$\boldsymbol{FC}$	[mm]	Water holding capacity	100 - 1000
$\boldsymbol{LP}$	[-]	Fraction of soil saturation above which evaporation happens unlimited	0.05 - 0.5
BetaSeepage	[-]	Non-linear exponent for soil store runoff generation	0.01 - 5.5
$\boldsymbol{k_s}$	[1/day]	Recession coefficient discharge from soil store	0.000001 - 0.5
		Groundwater storage	
$\boldsymbol{k_g}$	[1/day]	Recession coefficient for discharge from groundwater store	0.0008 - 0.1
$\boldsymbol{k_{sat}}$	[mm/day]	Recession coefficient for discharge from groundwater store	0.0008 - 5.0
$\boldsymbol{C_{flux}}$	[mm/day]	Capillary rise from groundwater module to soil store	0.05 - 0.5
$\boldsymbol{GW_{max}}$	[mm]	Maximum groundwater storage	1 - 2000
		Routing process	
$\boldsymbol{n}$	[-]	Manning coefficient	Water, Channels: 0.025 Forest: 0.2 Pasture: 0.259 Shrub, Croplands: 0.259 Urban: 0.013

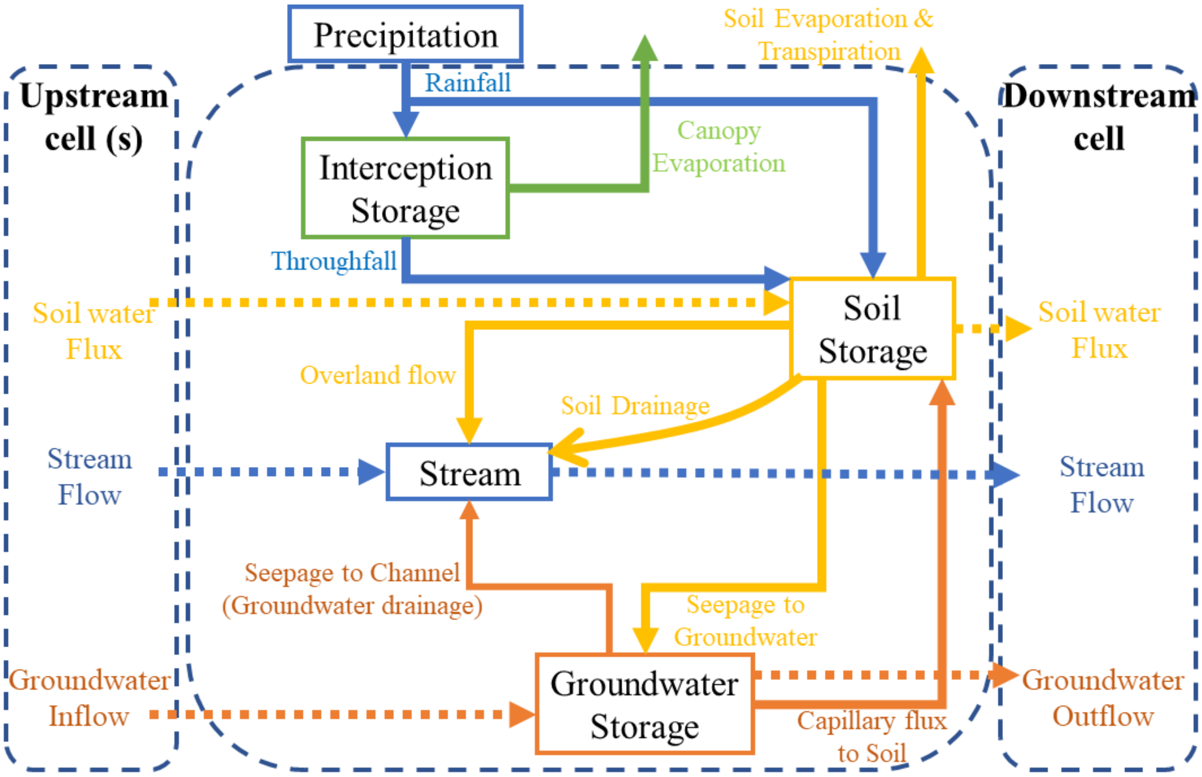

Figure S1. Model structure and key components in the modified STARR model

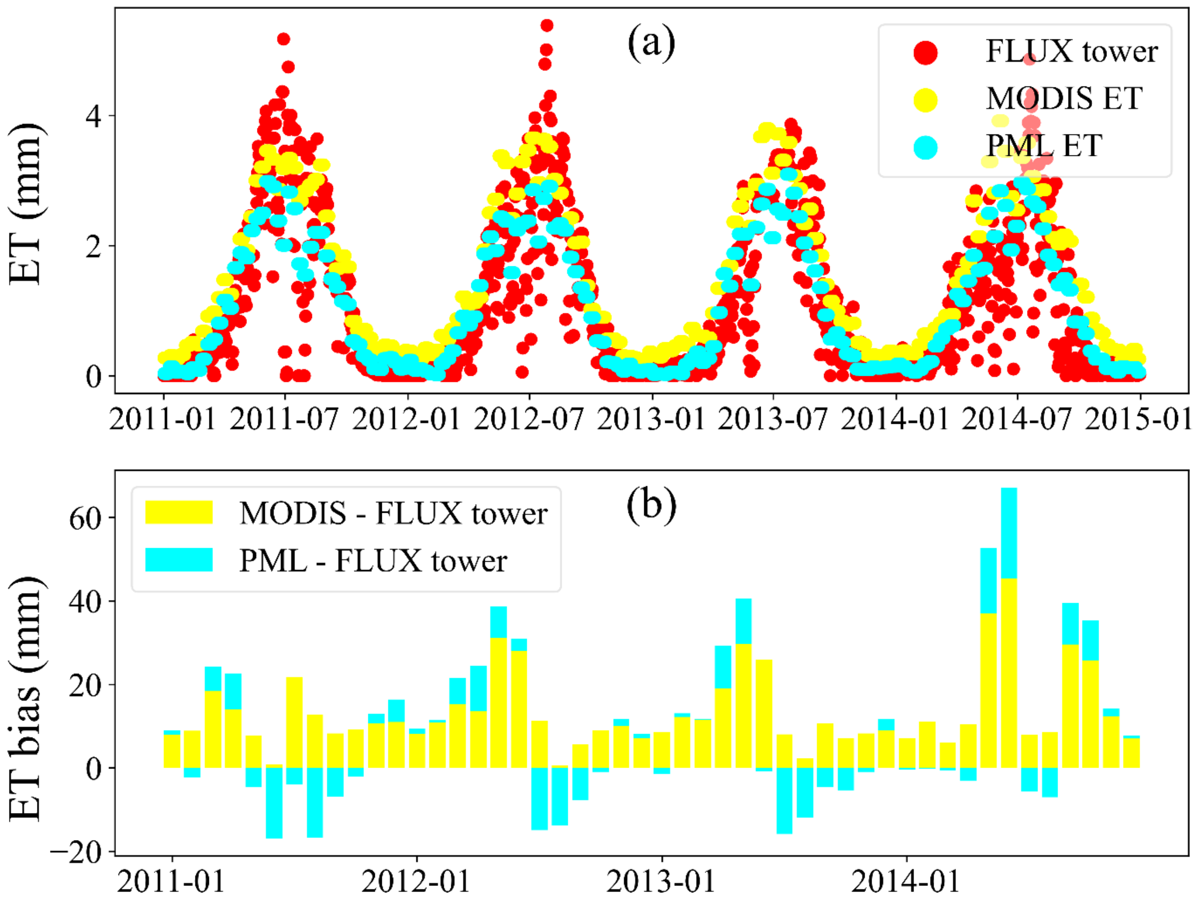

Figure S2. Comparison of ET between a Flux tower (51.8922 N, 14.0337 E), *MODIS and PML ET in the Spreewald. (a) Daily ET from Flux tower and 8-day ET from MODIS and PML; (b) Biased ET values between MODIS or PML and the Flux tower.*

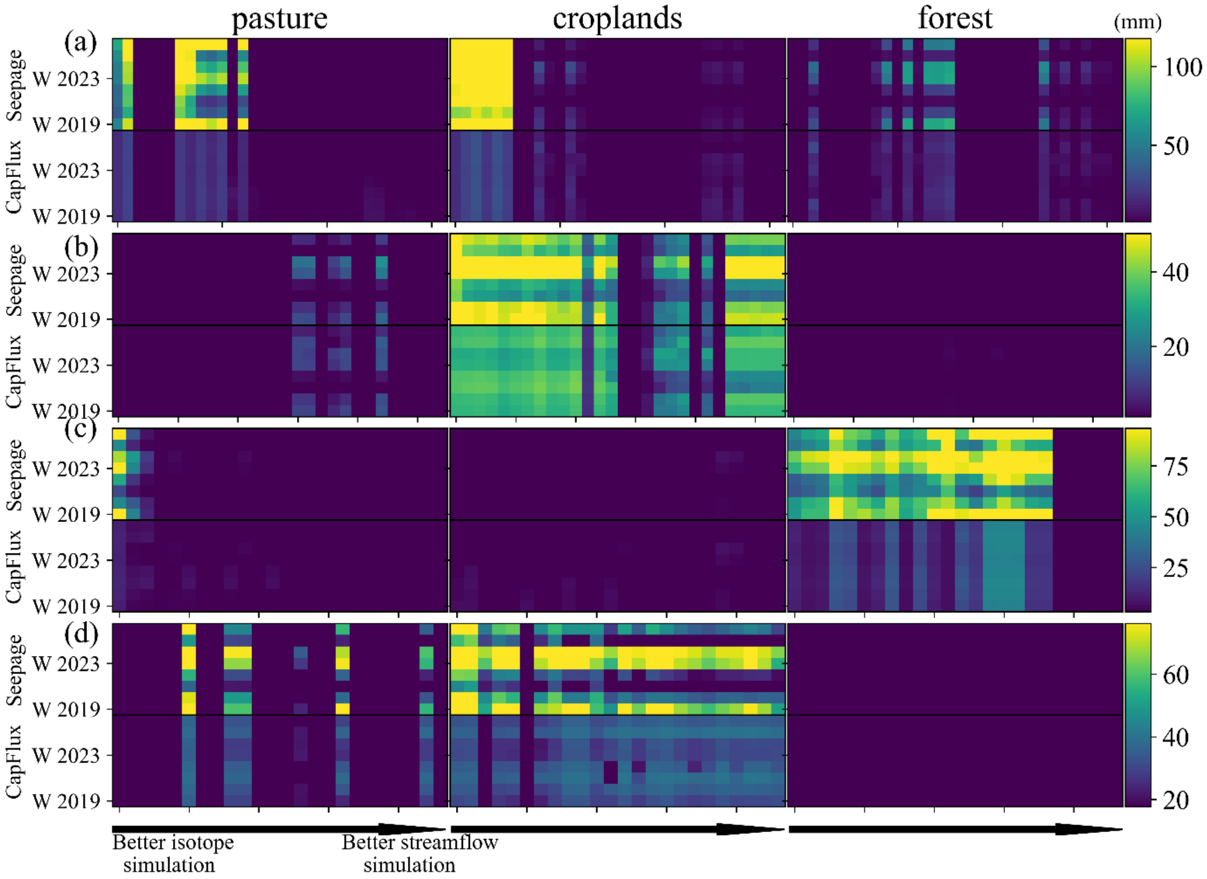

Figure S3. Total seasonal amount of runoff for different components, land uses and sub-catchments during 2019 and 2023 (winter, spring, summer, fall of 2019 and 2023 along Y-axis from bottom up, and "W" in the Y-label means winter) in the first Pareto front of (a) Bruckendorf (scheme 2); (b) Ragow (scheme 3); (c) Vetschau (scheme 4); (d) Boblitz (scheme 5). "Seepage" and "CapFlux" means soil seepage to groundwater and capillary flux from groundwater to soil storage, respectively. Each pixel in the plot is the total seasonal amount. X axis from left to right represents from the simulation with best simulated isotope to streamflow.

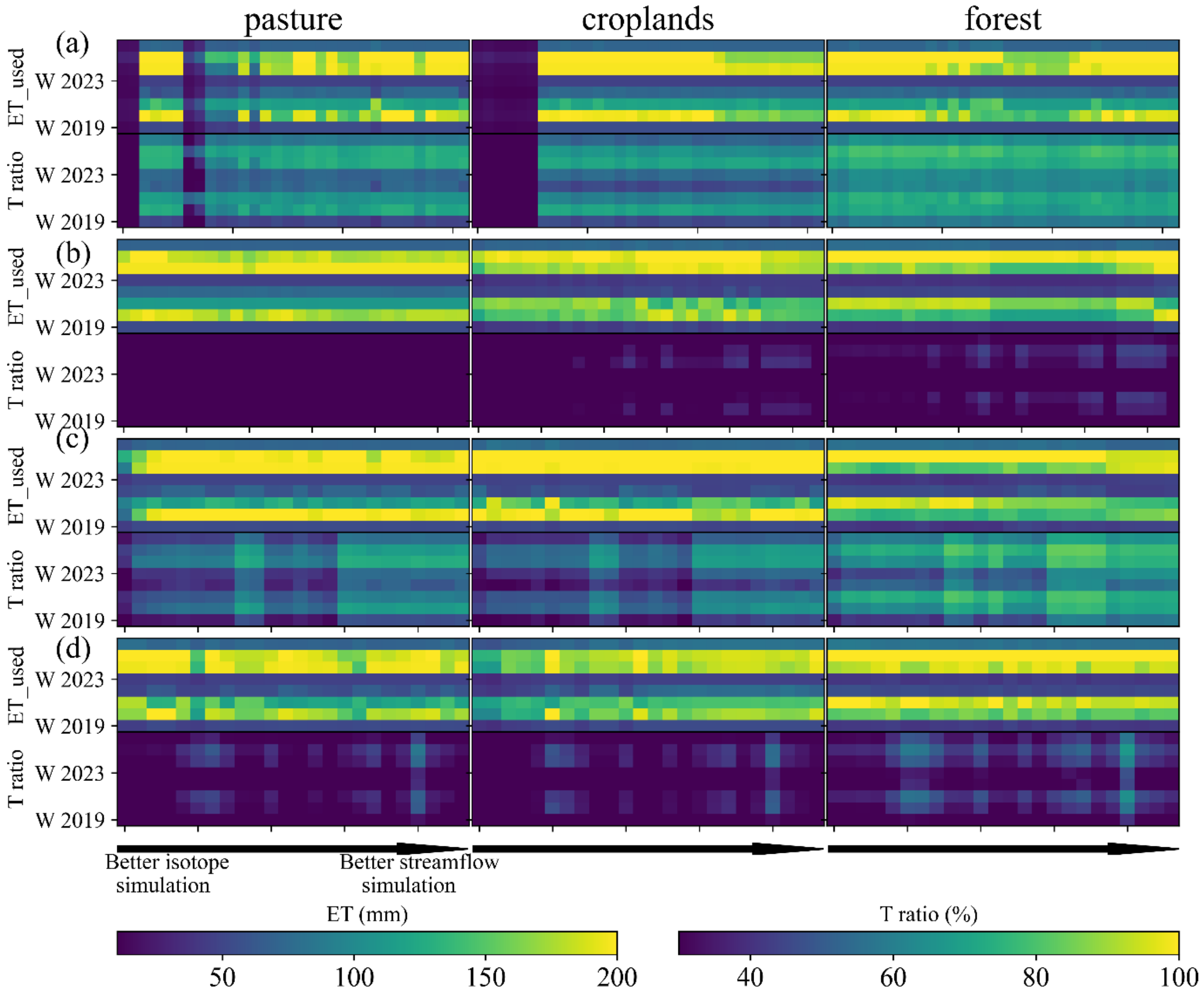

Figure S4. Total seasonal ET for different components, land uses and sub-catchments during 2019 and 2023 (winter, spring, summer, fall of 2019 and 2023 along Y-axis from bottom up, and "W" in the Y-label means winter) in the first Pareto front of (a) Berste (scheme 2); (b) Wudritz (scheme 3); (c) Vetschauer (scheme 4); (d) Dobra (scheme 5). "ET_used" and "T ratio" means ET and transpiration proportion in ET, respectively. Each pixel in the plot is the total seasonal amount. X axis from left to right represents from the simulation with best simulated isotope to streamflow.