

Article

Chain Decomposition Reveals Precipitation-Sensitive Patterns of Ecosystem Carbon–Water Coupling in Karst and Non-Karst Landscapes of Southwest China

Yutao He ^{1,2}, Shadong Qu ^{3,4}, Suihua Liu ^{1,2,*} and Man Li ^{1,2,*}

¹ School of Geography and Environmental Sciences, Guizhou Normal University, Guiyang 550025, China; sy0230@gznu.edu.cn

² Key Laboratory of Remote Sensing Applications in Mountain Resources and Environment, Guiyang 550025, China

³ Key Laboratory of Mountain Hazards and Engineering Resilience, Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, Beijing 100101, China; qushadong0036@igsrr.ac.cn

⁴ University of Chinese Academy of Sciences, Beijing 100049, China

* Correspondence: lsh23h@gznu.edu.cn (S.L.); 201508042@gznu.edu.cn (M.L.)

Abstract

Precipitation use efficiency (PUE) links ecosystem carbon uptake to precipitation input, but endpoint ratios alone cannot show where carbon–water coupling differs along ecohydrological pathways. This limitation is especially relevant in karst landscapes, where thin soils and heterogeneous hydrological pathways can decouple rainfall, soil moisture, evapotranspiration, and plant carbon gain. Here, we developed a PUE chain decomposition framework based on gross primary productivity (GPP), transpiration (T), evapotranspiration (ET), soil moisture (SM), and precipitation (PRE): $PUE = GPP/T \times T/ET \times ET/SM \times SM/PRE$. In this framework, GPP/T represents carbon fixation per unit transpiration, T/ET the transpiration fraction of evapotranspiration, ET/SM evapotranspiration output relative to soil moisture, and SM/PRE soil moisture status relative to precipitation input. We used multi-source remote-sensing and reanalysis data from 2003 to 2022 to compare karst and non-karst landscapes in Southwest China, applied variance decomposition to quantify the contributions of chain terms and their interactions, and used Stacking ensemble learning with Shapley additive explanations (SHAP) to interpret model-inferred environmental associations. Mean PUE was $1.16 \text{ g C m}^{-2} \text{ mm}^{-1}$ in non-karst areas and $1.08 \text{ g C m}^{-2} \text{ mm}^{-1}$ in karst areas, and all four chain components differed significantly between landform types. Variance decomposition identified SM/PRE and its interaction terms as the largest contributors to PUE variability, mainly reflecting a precipitation-sensitive diagnostic signal and soil moisture status relative to precipitation input. Machine learning interpretation showed that solar radiation, leaf area index, aridity, and groundwater storage were associated with different chain components; karst areas showed stronger groundwater-storage signals and lower model-inferred response thresholds. These findings indicate that PUE differences in Southwest China arise from multiple linked diagnostic stages rather than from endpoint carbon uptake or precipitation alone. The framework can help locate water-use constraints and support landform-specific ecological restoration and water management.

Academic Editors: Haijun Deng, Jianhua Xiao, Panxing He and Jiejie Sun

Received: 1 June 2026

Revised: 8 July 2026

Accepted: 9 July 2026

Published: 10 July 2026

Copyright: © 2026 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the [Creative Commons Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

Keywords: precipitation use efficiency; carbon–water coupling; karst landscape; soil moisture; machine learning; SHAP

1. Introduction

Global climate change is reshaping the balance between terrestrial carbon uptake and ecosystem water availability [1–3]. Vegetation greening and rising productivity can enhance terrestrial carbon uptake, but their hydrological effects are regulated by vegetation physiology and atmospheric demand. These controls include canopy structure, stomatal regulation, root-zone water availability, vapor pressure deficit, radiation, and temperature. Through these pathways, productivity changes may influence evapotranspiration, soil moisture, regional hydrological cycling, and land–atmosphere exchanges. Consequently, increases in carbon uptake can be associated with stronger carbon–water trade-offs, particularly where water availability constrains ecosystem recovery [4,5]. This issue is especially important in vulnerable land ecosystems with complex landforms and hydrological conditions.

Recent advances in multi-source remote sensing, reanalysis, and hydrological datasets now make it possible to track key ecohydrological variables, including vegetation productivity, precipitation, soil moisture, and evapotranspiration, over broad areas and long time periods. These data provide a basis for evaluating vegetation–hydrology–climate responses and their effects on ecosystem carbon–water coupling [3,6]. In this context, precipitation use efficiency (PUE), commonly defined as the ratio of gross primary productivity (GPP) to concurrent precipitation (PRE), is widely used to describe how effectively ecosystems convert precipitation input into carbon fixation [7–10]. Yet conventional PUE mainly captures the endpoint relationship between precipitation and productivity. Interpreting PUE only through the GPP/PRE ratio does not show how rainfall supports carbon fixation after passing through soil moisture maintenance, evapotranspiration output, and vegetation transpiration. It also makes it difficult to identify the process-level sources of water-use differences among land ecosystems [9,11–14].

Several water-use efficiency indicators describe carbon–water relations from different parts of the hydrological cycle. Water-use efficiency (WUE), usually calculated as GPP divided by evapotranspiration (ET), links ecosystem carbon uptake with total water loss [2,15,16]. It has also been separated into carbon fixation per unit transpiration (GPP/T) and the transpiration fraction of evapotranspiration (T/ET), which helps distinguish plant carbon gain from the partitioning of ET [15,17]. Soil water-use efficiency (SWUE), calculated as GPP/SM, shifts the focus to soil moisture as the water pool most directly available to vegetation [8,9]. PUE takes a different starting point. By using precipitation as the denominator, it asks how much carbon fixation is supported by rainfall input [7–10]. These indicators should not be treated as separate ways of describing unrelated processes. They look at the same carbon–water relationship from different positions along the water pathway: evapotranspiration loss, soil moisture storage, and precipitation input. This connection is important for PUE analysis because the GPP/PRE ratio is only the final expression of a longer process. Rainfall must first be retained as soil moisture, released through evapotranspiration, partitioned into transpiration, and then linked to carbon fixation. Reading WUE, SWUE, and PUE together therefore provides a basis for examining how PUE is formed through connected ecohydrological stages.

WUE, SWUE, and PUE have provided useful ways to describe ecosystem carbon–water relations, but they are still often treated as separate indicators. Many studies have also focused on statistical links between PUE and climatic, hydrological, or vegetation factors, with less attention to how these efficiency metrics are connected within a contin-

uous ecohydrological process. For PUE, which begins with precipitation input, the formation process is not a simple correspondence between rainfall amount and GPP. It includes a sequence of stages: precipitation input, soil moisture maintenance, evapotranspiration output, transpiration partitioning, and carbon gain per unit transpiration [2,11–17]. Previous studies have shown that PUE varies among ecosystems, climatic settings, and vegetation types, and it has been widely investigated in water-limited regions such as arid and semi-arid grasslands and the Loess Plateau [7,8,10]. However, the specific ecohydrological gap in humid karst landscapes remains insufficiently resolved. In these regions, the key question is not only how much precipitation enters the system, but how that water is retained, redistributed, and accessed by vegetation after rainfall [18,19]. This question becomes especially important under wet and dry climate anomalies, because thin soils, shallow soil reservoirs, exposed bedrock, and connected fissure–conduit networks can decouple monsoon precipitation from stable root-zone water supply [18]. During humid periods, rainfall may be rapidly lost through surface runoff, preferential infiltration, gravitational drainage, and subsurface leakage. During dry periods, vegetation water status may depend more strongly on antecedent soil moisture, delayed subsurface storage, groundwater access where available, and lithological controls on water retention [18–20]. Therefore, drought and humid scenarios may involve different limiting stages along the precipitation–soil moisture–evapotranspiration–transpiration–carbon gain chain.

The karst region of Southwest China provides a representative setting for examining this issue. Although monsoon precipitation is high, thin soils and well-developed karst systems, including fissures, sinkholes, and conduits, create strong spatial and temporal heterogeneity in precipitation retention, soil moisture maintenance, subsurface water availability, and vegetation growth conditions [18–21]. As a result, similar precipitation inputs may correspond to different soil moisture storage, evapotranspiration pathways, vegetation water use, and carbon uptake between karst and non-karst landscapes. In this setting, the conventional GPP/PRE ratio alone cannot distinguish whether PUE variation is associated with vegetation productivity, soil moisture status, evapotranspiration, transpiration partitioning, or precipitation variability. A PUE chain decomposition framework is therefore needed as a diagnostic approach to examine the intermediate terms linking precipitation input and ecosystem carbon gain across landform backgrounds and drought–humid conditions. Such an approach can provide a clearer basis for assessing water limitation and supporting ecological restoration and agricultural water management in vulnerable humid karst ecosystems.

In view of the above, this study takes Southwest China as the study area and constructs a PUE chain decomposition framework to diagnose the intermediate links between precipitation input and carbon fixation using multi-source remote sensing, reanalysis, and hydrological data. We compare the spatiotemporal patterns of PUE and its chain components between karst and non-karst areas and quantify their relative contributions to PUE variability. Because the environmental responses of PUE chain components in humid karst landscapes may be nonlinear, threshold-dependent, and scenario-specific, traditional linear or correlation-based methods may not fully characterize these relationships. We therefore combine Stacking ensemble learning with SHAP analysis to examine the model-inferred importance, response thresholds, and interaction patterns of environmental factors under drought and humid conditions. Specifically, this study aims to address three questions: (1) What are the spatiotemporal patterns of PUE and its chain components in karst versus non-karst areas of Southwest China? (2) Which chain components and interaction terms contribute most to PUE variability? (3) How do the model-inferred response thresholds and interaction patterns of environmental factors differ between karst and non-karst areas under drought versus humid conditions?

2. Materials and Methods

2.1. Study Area

The study area covers Yunnan Province, Guizhou Province, and Guangxi Zhuang Autonomous Region, which together form a typical humid karst region in Southwest China (Figure 1a) [22]. Situated on the Yunnan–Guizhou Plateau and its transitional zone toward the Guangxi hilly basins, this region represents one of the most concentrated and typically developed karst landscape areas in China. The overall topography is dominated by mountainous, plateau, and hilly landforms, with elevations generally increasing from the southeast to the northwest (Figure 1b). The region is under a subtropical humid monsoon climate, with relatively abundant precipitation. However, due to the thin soil layers in karst areas and the well-developed bedrock fractures and subsurface conduits, the retention of precipitation in surface and root-zone soil reservoirs is subject to considerable uncertainty [18,23,24]. Based on the datasets used in this study, the multi-year mean growing-season total precipitation during 2003–2022 was approximately 1078 mm (Figure 1d), and the corresponding mean growing-season GPP was approximately 1145 g C m⁻² (Figure 1c).

To compare the differences in intermediate processes of precipitation use efficiency between karst and non-karst areas under different moisture conditions, this study defined drought and humid scenarios based on the 12-month Standardized Precipitation Evapotranspiration Index (SPEI-12) (Figure 1e). According to the dry–wet classification scheme of SPEI, values between −0.5 and 0.5 indicate normal conditions, values below −0.5 indicate dry conditions, and values above 0.5 indicate wet conditions [25]. A year was defined as a drought scenario year when the SPEI-12 values of both karst and non-karst areas were below −0.5, and as a humid scenario year when the SPEI-12 values of both areas exceeded 0.5. Consequently, 2003, 2009, 2011, and 2021 were selected as drought scenario years, and 2008, 2015, and 2017 were selected as humid scenario years for comparative analysis.

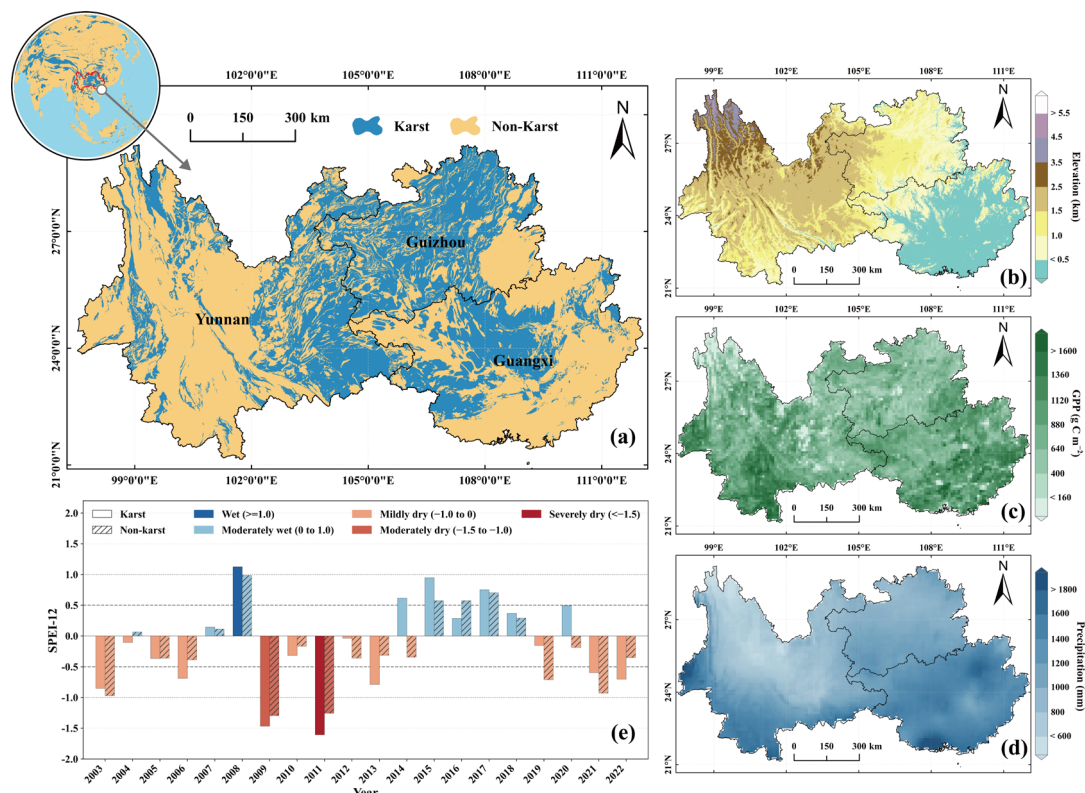


Figure 1. Overview of the study area. (a) Distribution of karst and non-karst areas; (b) elevation; (c) multi-year mean growing-season total GPP during 2003–2022; (d) multi-year mean growing-season

total precipitation during 2003–2022; (e) interannual variations in SPEI-12 in karst and non-karst areas.

2.2. Data and Preprocessing

The datasets used in this study fall into two groups: ecohydrological variables for constructing PUE and its chain components, and environmental driving factors covering meteorological, hydrological, vegetation, and topographic domains. Table 1 summarizes the main characteristics of all datasets.

For the ecohydrological variables, GPP, vegetation transpiration (T), and actual evapotranspiration (ET) were obtained from PML_V2 (Penman–Monteith–Leuning version 2). This product estimates GPP, ET, and ET components by combining the Penman–Monteith–Leuning model with remotely sensed vegetation parameters and meteorological forcing [26]. Its ET estimates have been shown to agree well with eddy-covariance flux tower observations, including in humid and semi-humid regions of China [27]. Soil moisture (SM) was taken from SMC1.0 (Soil Moisture of China by In Situ Data, version 1.0). SMC1.0 combines ground observations with ancillary datasets, including ERA5-Land, to provide daily 1 km soil moisture across China for 2000–2022 over the 0–1 m soil profile [28]. The product has been evaluated against field measurements [28]. In Southwest China, Zheng et al. (2025) compared SMC1 soil moisture with observations from 37 monitoring stations in Yunnan Province and reported reliable performance in karst terrain [19]. In this study, the 0–1 m profile-mean volumetric soil moisture ($\text{m}^3\cdot\text{m}^{-3}$) was converted to soil water storage (mm) by multiplying by the soil profile depth of 1000 mm. Precipitation (PRE) was obtained from MSWEP V2.8 (Multi-Source Weighted-Ensemble Precipitation version 2.8). MSWEP merges gauge, satellite, and reanalysis precipitation data, with bias correction and station-based constraints, to produce long-term precipitation fields at high spatiotemporal resolution [29]. Evaluation studies have reported stable performance in humid China, western mountainous terrain, and mountain regions of Southwest China [30–32]. We therefore used MSWEP as the precipitation input for calculating PUE and its chain components.

Table 1. Overview of datasets employed in this research.

Product	Variables	Spatial Resolution	Source
PML_V2 [26]	GPP	500 m	https://developers.google.com/earth-engine/datasets/catalog/CAS_IGSNRR_PML_V2_v018 (accessed on 26 April 2026)
	T		
	ET		
SMCI [28,33]	SM	1 km	https://doi.org/10.11888/Terre.tpd.272415 (accessed on 23 April 2026)
MSWEP [29]	PRE	0.1°	https://www.gloh2o.org/mswep/ (accessed on 6 February 2026)
ERA5-Land [34]	Wind	0.1°	https://cds.climate.copernicus.eu/datasets (accessed on 10 April 2026)
	SRAD		
	TMP		
GLEAM [35]	PET	0.1°	https://www.gleam.eu/ (accessed on 14 April 2026)
GloFAS [36]	Runoff	0.1°	https://ewds.climate.copernicus.eu/datasets (accessed on 22 March 2026)
HWSA [37,38]	GWSA	0.05°	https://doi.org/10.11888/Terre.tpd.300962 (accessed on 27 March 2026)
GLASS [39]	LAI	0.05°	https://glass.hku.hk/ (accessed on 27 March 2026)
MERIT [40,41]	Elevation	~90 m	https://global-hydrodynamics.github.io/ (accessed on 16 January 2026)

CHM_Drought [42]	SPEI-12	0.1°	https://zenodo.org/records/14634774 (accessed on 30 March 2026)
CLCD [43]	Land use	30 m	https://zenodo.org/records/18180184 (accessed on 11 February 2026)

Environmental driving factors span four categories. Among the meteorological factors, surface solar radiation downwards (SRAD), 2 m air temperature (TMP), and wind speed (Wind) were extracted from ERA5-Land reanalysis data (~0.1° resolution) [34]. The aridity index (AI) was calculated as the ratio of precipitation (PRE) to potential evapotranspiration (PET), with PET sourced from the GLEAM dataset [35]. In this study, AI represents the relative balance between atmospheric water supply and potential evaporative demand; therefore, higher AI values indicate wetter conditions, whereas lower AI values indicate drier conditions. Vapor pressure deficit (VPD) was derived from ERA5-Land 2 m air temperature and 2 m dewpoint temperature as follows [44]:

$$e_s = 0.611 \times \exp\left(\frac{17.27T}{T+237.29}\right) \quad (1)$$

$$e_a = 0.611 \times \exp\left(\frac{17.27T_d}{T_d+237.29}\right) \quad (2)$$

$$VPD = e_s - e_a \quad (3)$$

where T is the 2 m air temperature (°C) and T_d is the 2 m dewpoint temperature (°C).

Hydrological factors include runoff equivalent and groundwater storage anomaly. Runoff equivalent data were obtained from the Global Flood Awareness System (GloFAS) historical hydrological dataset, which drives the LISFLOOD hydrological model with ERA5 meteorological reanalysis to generate global-scale hydrological variables [36]. Groundwater storage anomaly (GWSA) data come from the high-resolution water storage anomaly dataset (HWSA v1.0). This product downscales GRACE/GRACE-FO Mascon data to 0.05° monthly resolution (April 2002–December 2022) through a physics-constrained sliding-window framework (MLDF-PCSW) [37]; its estimates maintain high consistency with original Mascon products and agree well with in situ groundwater observations [37]. Vegetation conditions were represented by leaf area index (LAI) from the GLASS (Global Land Surface Satellite) dataset. We used the GLASS V6 LAI product, which is generated from MODIS observations with a bidirectional long short-term memory network (Bi-LSTM). Previous validation has shown that the product has good accuracy and temporal continuity [39]. Topographic variables included elevation, slope, topographic wetness index (TWI), and aspect. Elevation was obtained from MERIT DEM, a global elevation dataset at approximately 90 m resolution that reduces major error components in earlier satellite DEMs [40]. Slope and aspect were calculated from MERIT DEM. TWI was derived using hydrological terrain attributes from MERIT Hydro [41]. Because aspect is a circular variable, aspect angles were transformed into $\sin(\text{Aspect})$ and $\cos(\text{Aspect})$, hereafter referred to as ASPsin and ASPcos. The 12-month Standardized Precipitation Evapotranspiration Index (SPEI-12), used to classify drought and humid scenarios, was obtained from the China High-resolution Multi-Drought Index dataset (CHM_Drought) [42]. The karst/non-karst classification was derived from the 1:500,000 Karst Hydrogeological Map provided by GeoCloud, China Geological Survey (<https://geocloud.cgs.gov.cn/>). Carbonate rock and karst hydrogeological units were classified as karst areas, while other lithological or non-karst hydrogeological units were classified as non-karst areas.

Before analysis, all datasets were harmonized to a common 0.1° analysis grid using spatial aggregation. Variables with native spatial resolutions finer than 0.1° were spatially

aggregated to 0.1°. For continuous variables, the mean value of all valid pixels within each 0.1° grid cell was used; for categorical variables, the dominant category within each 0.1° grid cell was assigned. All datasets were then clipped to the study area. Variables with different native temporal resolutions were first aggregated to monthly values and then further aggregated to growing-season annual values, with the growing season defined as April to October. Because water-use efficiency indicators are mainly meaningful for vegetated ecosystems, non-vegetated areas were excluded using the China Land Cover Dataset (CLCD) [43].

2.3. Methods

The overall analytical framework of this study is illustrated in Figure 2.

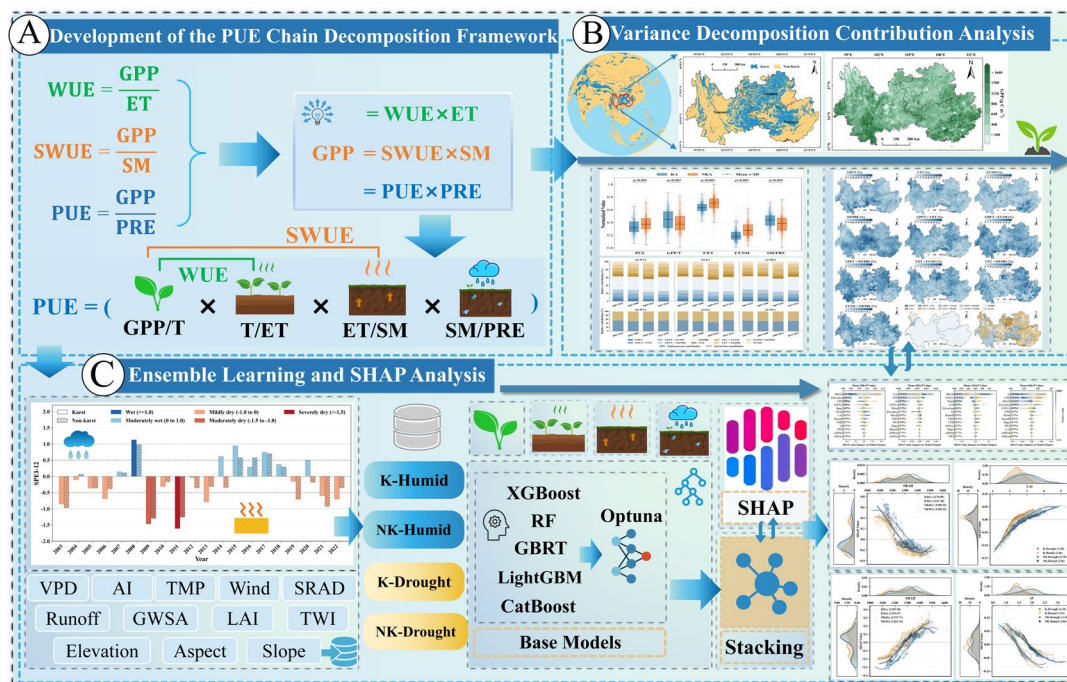


Figure 2. Overview of the analytical framework employed in this study. (A) Derivation and formulation of the PUE chain decomposition framework. (B) Variance decomposition of chain-component contributions to PUE. (C) Stacking ensemble learning combined with SHAP analysis for driving factor interpretation under drought and humid conditions in karst and non-karst areas.

2.3.1. Development of a PUE Chain Decomposition Framework

From precipitation input through evapotranspiration output to vegetation carbon fixation, ecosystem water utilization is a continuous process of water supply, retention, and conversion. In previous studies, PUE is commonly defined as the ratio of GPP to concurrent PRE, representing the carbon fixation capacity sustained per unit of precipitation input. Correspondingly, SWUE is defined as the ratio of GPP to soil water storage (SM), characterizing the carbon fixation capacity associated with per unit of soil water storage [8,9]. Their expressions are as follows:

$$\text{PUE} = \frac{\text{GPP}}{\text{PRE}} \quad (4)$$

$$\text{SWUE} = \frac{\text{GPP}}{\text{SM}} \quad (5)$$

where GPP denotes vegetation gross primary productivity ($\text{g C} \cdot \text{m}^{-2}$), PRE denotes precipitation (mm), and SM denotes soil water storage (mm).

From Equations (4) and (5), it follows that:

$$GPP = PUE \times PRE = SWUE \times SM \quad (6)$$

Therefore:

$$PUE = SWUE \times \frac{SM}{PRE} \quad (7)$$

In previous studies on water-use efficiency, conventional WUE is typically defined as the ratio of GPP to actual evapotranspiration. Some studies have further decomposed WUE into two process components: transpiration-based carbon fixation capacity and evapotranspiration partitioning [15–17], expressed as:

$$WUE = \frac{GPP}{ET} = \frac{GPP}{T} \times \frac{T}{ET} \quad (8)$$

where T denotes vegetation transpiration (mm) and ET denotes actual evapotranspiration (mm). Building upon this, by further introducing the soil moisture term, SWUE can be expressed as:

$$SWUE = \frac{GPP}{T} \times \frac{T}{ET} \times \frac{ET}{SM} \quad (9)$$

Substituting Equation (9) into Equation (7) yields the PUE chain decomposition formulated in this study:

$$PUE = \frac{GPP}{T} \times \frac{T}{ET} \times \frac{ET}{SM} \times \frac{SM}{PRE} \quad (10)$$

In this formulation, GPP/T denotes carbon fixation per unit transpiration, and T/ET denotes the share of transpiration in total evapotranspiration. ET/SM describes evapotranspiration output relative to the soil moisture pool, whereas SM/PRE describes the soil moisture condition associated with precipitation input. This multiplicative formulation was adopted because PUE is defined as GPP/PRE and can therefore be algebraically rearranged into intermediate ratios linking precipitation, soil moisture, evapotranspiration, transpiration, and carbon fixation while preserving the mathematical identity of PUE. It also places WUE, SWUE, and PUE within a common diagnostic framework, in which precipitation input, soil moisture status, evapotranspiration output, transpiration partitioning, and transpiration-based carbon fixation are treated as connected diagnostic stages rather than separate ratios. In this framework, ET/SM and SM/PRE are interpreted as pixel-scale diagnostic proxy terms that describe relative variation between adjacent stages, rather than as physically strict efficiency metrics or direct evidence of water-transfer processes. Compared with structural equation modeling (SEM), which is more suitable for testing predefined causal pathways and indirect effects, this identity-based framework is better suited to diagnosing how PUE variability is distributed among adjacent terms without imposing an a priori causal path structure [45].

2.3.2. Trend Analysis and Breakpoint Identification

To identify the trends and stage-specific characteristics of PUE variations during the study period, this study combined linear trend analysis, the coefficient of variation (CV), and breakpoint detection to quantitatively analyze the temporal dynamics of PUE. The linear trend was estimated using ordinary least squares (OLS) regression:

$$PUE_t = \beta_0 + \beta_1 \cdot t + \varepsilon_t \quad (11)$$

where β_1 is the trend slope, representing the mean annual rate of change in PUE. The statistical significance of the slope was assessed using a two-tailed t-test, and the coeffi-

coefficient of determination R^2 was used to evaluate the goodness of fit. The significance level was set at $\alpha = 0.05$.

The coefficient of variation (CV) is defined as the ratio of the standard deviation to the mean:

$$CV = \frac{\sigma}{\bar{x}} \times 100\% \quad (12)$$

Higher CV values indicate stronger interannual fluctuations in PUE and lower temporal stability. For breakpoint detection, the optimal breakpoint was determined by minimizing the residual sum of squares (SSE), while jointly considering regional conditions and the trend characteristics, significance levels, R^2 , and CV of each sub-period.

2.3.3. Variance Decomposition of Chain-Process Contributions

The PUE chain decomposition framework separates the continuous process from precipitation input to carbon fixation into four sequential components. To quantify the relative contributions of each component to the temporal variability in PUE and to distinguish between the variance contributions of individual components and the covariance contributions among components, this study employed a variance–covariance decomposition method based on first-order total differential approximation [45]. According to the multiplicative structure of PUE in Equation (10):

$$PUE_t = R_{1,t} \cdot R_{2,t} \cdot R_{3,t} \cdot R_{4,t} \quad (13)$$

where

$$R_1 = GPP/T, \quad R_2 = T/ET, \quad R_3 = ET/SM, \quad R_4 = SM/PRE \quad (14)$$

During the study period, using the temporal mean $\bar{R}_k$ of each variable as the expansion point for first-order total differential approximation, the interannual anomaly of PUE can be approximately expressed as a linear superposition of the anomalies of each variable:

$$\Delta PUE_t \approx \sum_{k=1}^4 g_k \cdot \Delta R_{k,t} \quad (15)$$

where $\Delta R_{k,t}$ is the anomaly of the k -th chain component in year t relative to the multi-year mean, and g_k is the partial derivative coefficient evaluated at the mean values:

$$g_k = \left. \frac{\partial PUE}{\partial R_k} \right|_{\bar{R}_1, \bar{R}_2, \bar{R}_3, \bar{R}_4} \quad (16)$$

The partial derivatives can be expressed as:

$$g_1 = \bar{R}_2 \bar{R}_3 \bar{R}_4, \quad g_2 = \bar{R}_1 \bar{R}_3 \bar{R}_4, \quad g_3 = \bar{R}_1 \bar{R}_2 \bar{R}_4, \quad g_4 = \bar{R}_1 \bar{R}_2 \bar{R}_3 \quad (17)$$

Accordingly, the temporal variance of PUE can be decomposed into the sum of independent variance terms of each chain component and pairwise covariance interaction terms:

$$\text{Var}(PUE) \approx \sum_{k=1}^4 g_k^2 \text{Var}(R_k) + 2 \sum_{1 \leq k < l \leq 4} g_k g_l \text{Cov}(R_k, R_l) \quad (18)$$

where $\text{Var}(R_k)$ is the unbiased sample variance of the k -th chain variable, and $\text{Cov}(R_k, R_l)$ is the unbiased sample covariance between any two chain variables.

The variance contribution of the k -th process is further defined as:

$$C_k = g_k^2 \cdot \text{Var}(R_k) \quad (19)$$

The covariance contribution between the k -th and l -th chain components is defined as:

$$C_{kl} = 2g_k g_l \text{Cov}(R_k, R_l) \quad (20)$$

where $C_{kl} > 0$ indicates that co-directional variations between the two processes amplify PUE fluctuations, and $C_{kl} < 0$ indicates that opposing variations between the two processes dampen PUE fluctuations. To avoid underestimation of contribution magnitudes caused by the cancelation of positive and negative terms, the relative contribution (RC) was calculated using absolute-value normalization:

$$RC_k = \frac{|C_k|}{\sum_{k=1}^4 |C_k| + \sum_{1 \leq k < l \leq 4} |C_{kl}|} \times 100\% \quad (21)$$

$$RC_{kl} = \frac{|C_{kl}|}{\sum_{k=1}^4 |C_k| + \sum_{1 \leq k < l \leq 4} |C_{kl}|} \times 100\% \quad (22)$$

2.3.4. Stacking Modeling and Performance Evaluation

To identify the environmental driving factors of PUE chain components under different scenarios, this study constructed machine learning models for each of the four intermediate processes (GPP/T, T/ET, ET/SM, and SM/PRE) under four scenarios: karst-drought (K-Drought), karst-humid (K-Humid), non-karst-drought (NK-Drought), and non-karst-humid (NK-Humid), resulting in a total of 16 modeling cases. For each scenario, the response variables and predictor variables were calculated as scenario-specific multi-year means. The predictor variables include climatic factors (TMP, SRAD, VPD, Wind, AI), vegetation-hydrological factors (LAI, GWSA, Runoff), and topographic factors (Elevation, Slope, TWI, ASPsin, ASPcos), comprising 13 feature variables in total.

The combined framework of machine learning and SHAP has been widely applied in earth science research, providing an effective tool for identifying important predictors and interpreting model outputs [46–50]. Because SHAP is primarily used for model interpretation, the choice of the underlying predictive model matters. To reduce model selection bias, five machine learning algorithms commonly used in earth science were selected as base learners: Random Forest (RF) [51], Extreme Gradient Boosting (XGBoost) [52], Light Gradient Boosting Machine (LightGBM) [53], CatBoost [54], and Gradient Boosted Regression Trees (GBRT) [55]. RF combines multiple decision trees to capture nonlinear relationships and variable interactions. GBRT builds regression trees sequentially to reduce residual errors. XGBoost improves gradient boosting through regularization and optimized computation. LightGBM uses histogram-based learning and leaf-wise tree growth to improve the efficiency of gradient-boosted decision trees. CatBoost uses ordered boosting to reduce prediction bias and improve model robustness [51–55]. A Stacking ensemble model was then built on top of these base learners [56,57]. For each modeling case, the samples were randomly divided into training, validation, and test sets at a ratio of 7:1:2. The machine learning analyses used 2812 valid pixel samples for karst areas and 3595 valid pixel samples for non-karst areas in each drought or humid scenario. To assess residual spatial dependence after model fitting, Moran's I values of the model residuals and effective sample size estimates were calculated and are reported in Supplementary Note S3.

In this study, the hyperparameters of each base learner were optimized using the Optuna framework [58], and model performance was evaluated on the test set using the coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE). On this basis, Ridge regression was employed as the meta-learner to further construct the Stacking ensemble model [59]. Let $\hat{y}_m$ denote the prediction of the m -th base learner; the Stacking model can be expressed as:

$$\hat{y}_{\text{stack}}(x) = \alpha + \sum_{m=1}^M \omega_m \hat{y}_m(x) \quad (23)$$

where α is the intercept term, ω_m is the weight coefficient of the m -th base learner, and $M = 5$. The performance of individual models and the Stacking model was compared on the test set using R^2 , RMSE, and MAE, and the model with the best overall performance was selected for subsequent interpretable analysis.

2.3.5. SHAP-Based Interpretation and Interaction Analysis

To reveal the influence direction, contribution magnitude, and potential nonlinear relationships of different environmental factors on the prediction results of PUE chain components, this study employed the Shapley Additive Explanations (SHAP) method for interpretable analysis of the machine learning models [60,61]. The SHAP value is calculated as follows:

$$\phi_j(v) = \sum_{S \subseteq \{1, \dots, p\} \setminus \{j\}} \frac{|S|!(p-|S|-1)!}{p!} (v_x(S \cup \{j\}) - v_x(S)) \quad (24)$$

where ϕ_j denotes the SHAP value of feature j , S is a subset of the features used by the model, and $v_x(S)$ represents the model prediction based solely on the feature subset S . $\phi_j > 0$ and $\phi_j < 0$ indicate positive and negative effects of feature j on the prediction result, respectively. We used SHAP values to rank the feature importance of environmental factors for each scenario and each chain component, and employed SHAP dependence plots to analyze the influence direction and potential threshold characteristics of key factors.

3. Results

3.1. Spatiotemporal Dynamics of PUE and Its Chain Components

Over 2003–2022, the multi-year means of PUE and its four chain components displayed pronounced regional differentiation across the study area (Figure 3). The area-averaged PUE was $1.13 \text{ g C m}^{-2} \text{ mm}^{-1}$, with an overall spatial pattern of higher values in the west and lower values in the east. At the provincial scale, the proportion of area with PUE values above the regional mean was 60.80% in Yunnan, 34.71% in Guizhou, and 20.82% in Guangxi. High-PUE zones were concentrated in central and northern Yunnan, while low-PUE zones were mainly distributed across southwestern Guizhou and northwestern Guangxi. The spatial distributions of the four chain components did not mirror that of PUE: high GPP/T and SM/PRE values occurred mainly in Guizhou and parts of Yunnan; high T/ET values were found in central–southern Yunnan, eastern Guangxi, and southwestern Guangxi; high ET/SM values were confined to localized areas of southern and northwestern Yunnan. These patterns indicate that the spatial pattern of PUE does not correspond to any single chain component but instead arises from the combined spatial heterogeneity of different chain components.

Comparisons between karst and non-karst areas further revealed significant differences in PUE and all four chain components, as indicated by the Mann–Whitney U tests shown in Figure 3f. Based on the statistics of original values, PUE in non-karst areas was significantly higher than that in karst areas, with mean values of 1.16 and $1.08 \text{ g C m}^{-2} \text{ mm}^{-1}$, respectively. GPP/T and SM/PRE were higher in karst areas (means of 3.74 and 0.41) than in non-karst areas (3.62 and 0.39), whereas T/ET and ET/SM were higher in non-karst areas (0.61 and 1.40) than in karst areas (0.58 and 1.24). To further explain the component sources of this PUE difference, we conducted a log-ratio mean decomposition in Supplementary Note S2. The results showed that the higher PUE in non-karst areas was mainly associated with positive contributions from T/ET and ET/SM, especially ET/SM, whereas

the relatively higher GPP/T and SM/PRE in karst areas partly offset the non-karst PUE advantage.

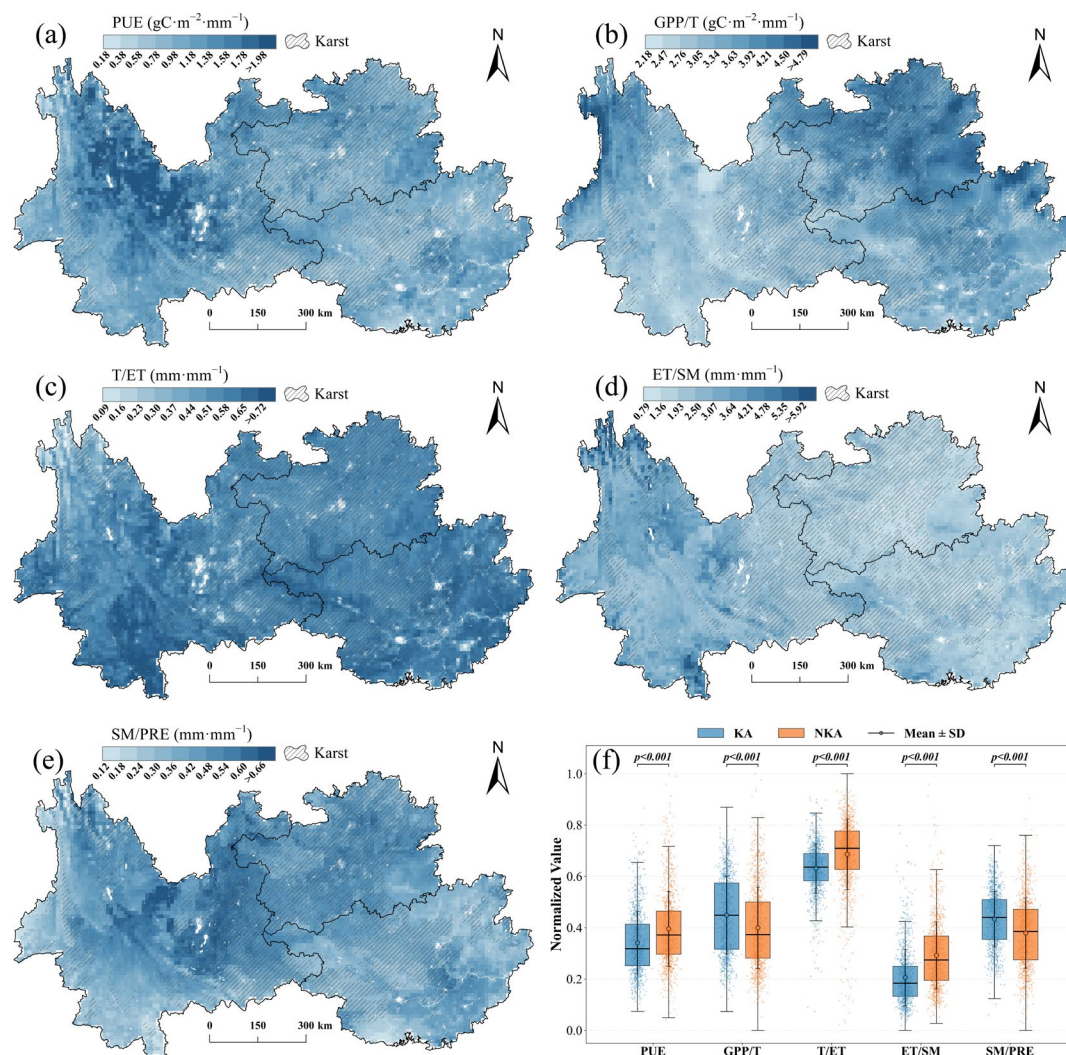


Figure 3. Spatial patterns of PUE and its chain components across the study area during 2003–2022. (a–e) Spatial distributions of the multi-year growing-season mean values of PUE, GPP/T, T/ET, ET/SM, and SM/PRE, respectively. (f) Standardized box plots comparing each indicator between the karst area (KA) and non-karst area (NKA), with annotations indicating p -values from the Mann–Whitney U test.

Temporally, growing-season PUE and its chain components fluctuated over 2003–2022, yet the amplitude and phase characteristics differed among components (Figure 4). PUE exhibited the most pronounced interannual variability, ranging from 0.97 to 1.44 $\text{g C m}^{-2} \text{mm}^{-1}$ across the study area. No clear monotonic trend was evident, although PUE in non-karst areas consistently exceeded that in karst areas. PUE peaked in 2011; the lowest values for the whole study area and non-karst areas both occurred in 2010, while that for karst areas occurred in 2014.

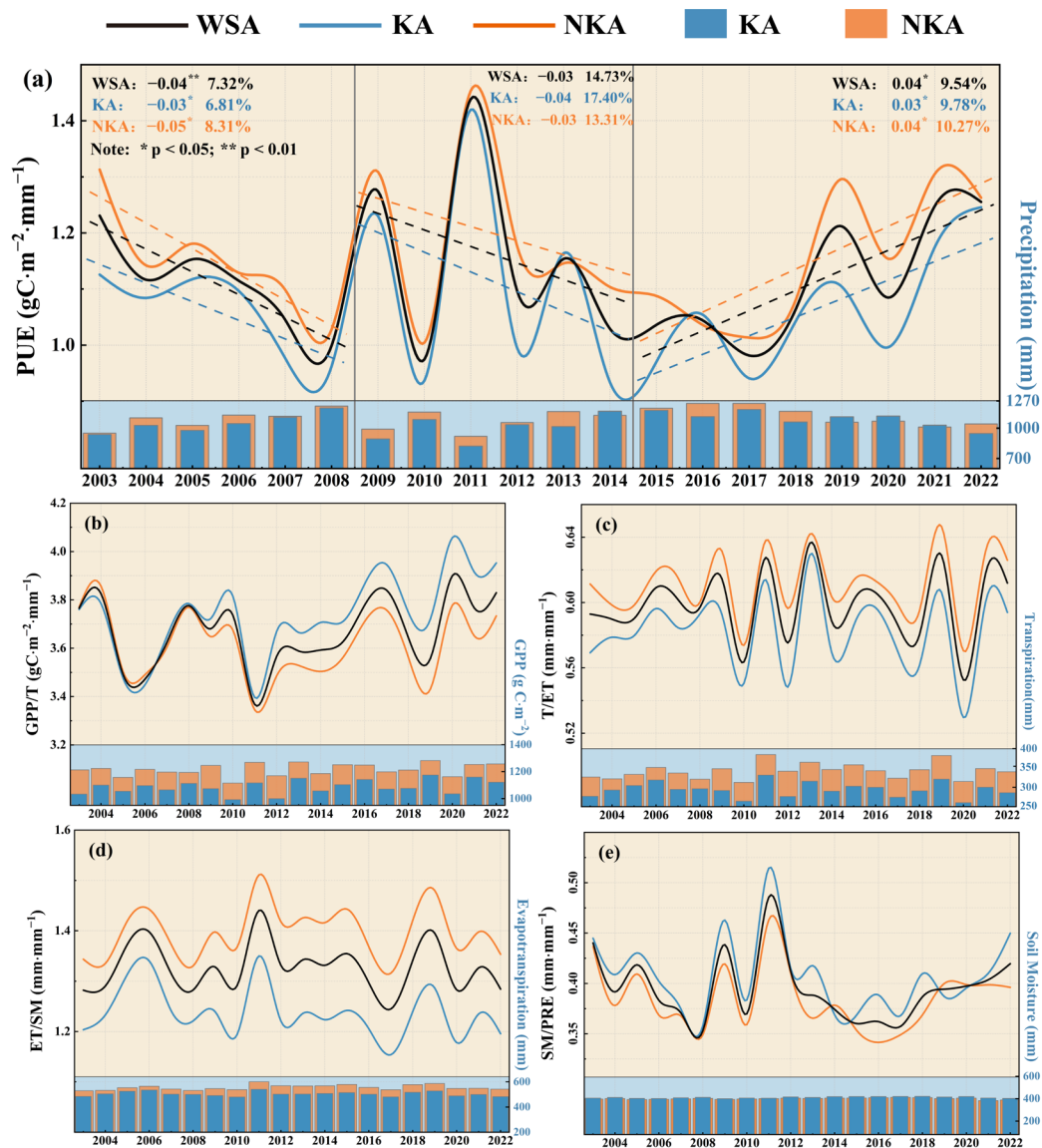


Figure 4. Temporal dynamics of PUE and its chain components across the study area during 2003–2022. (a–e) Interannual variations in PUE, GPP/T, T/ET, ET/SM, and SM/PRE for the whole study area (WSA), karst area (KA), and non-karst area (NKA), respectively, with curves fitted using spline smoothing. The lower panel of (a) shows the temporal variation in PRE, and the lower panels of (b–e) show the temporal variations in GPP, T, ET, and SM, respectively.

To characterize the stage-specific fluctuation pattern of PUE, we first applied automatic breakpoint detection based on the minimum SSE criterion (Table 2). This procedure identified 2010 and 2015 as statistical breakpoints in the PUE time series across the three regional subsets. However, because our objective was to interpret PUE changes in relation to regional hydroclimatic conditions, we further defined three hydroclimatic phases using the temporal evolution of SPEI-12: 2003–2008, 2009–2014, and 2015–2022. This phase division was not used to replace the statistical breakpoint detection, but to align the temporal analysis with the drought evolution shown in Figure 1e. SPEI-12 declined markedly from 2008 to 2009, and the 2009–2014 mean SPEI-12 values were -0.60 and -0.62 for karst and non-karst areas, respectively, indicating a relatively dry middle phase. Piecewise linear fitting based on this hydroclimatic phase division showed that PUE declined significantly during 2003–2008, with slopes of -0.0403, -0.0332, and -0.0459 yr⁻¹ for the whole study area, karst areas, and non-karst areas, respectively. PUE continued to decline during 2009–2014, although the trends were not statistically significant. During 2015–2022, PUE recov-

ered significantly, with slopes of 0.0358, 0.0328, and 0.0382 yr⁻¹. The coefficient of variation indicated that all three regional subsets experienced the strongest fluctuations during 2009–2014, with CV values of 14.73%, 17.40%, and 13.31%, respectively. Overall, PUE exhibited a three-phase temporal trajectory under the SPEI-informed hydroclimatic division: an initial decline, intensified fluctuations in the dry middle phase, and recovery growth in the later period.

Table 2. Comparison of stage-specific characteristics of PUE under different segmentation schemes across WSA, KA, and NKA.

Region	Scheme	Period	Trend	R ²	CV (%)
WSA	Auto-break	2003–2010	– (ns)	0.180	9.50
		2011–2015	– (ns)	0.669	14.66
		2016–2022	+ (*)	0.698	9.73
	Adjusted	2003–2008	– (**)	0.862	7.32
		2009–2014	– (ns)	0.104	14.73
		2015–2022	+ (*)	0.680	9.54
KA	Auto-break	2003–2010	– (ns)	0.118	9.38
		2011–2015	– (ns)	0.570	18.34
		2016–2022	+ (ns)	0.541	9.68
	Adjusted	2003–2008	– (*)	0.739	6.81
		2009–2014	– (ns)	0.115	17.40
		2015–2022	+ (*)	0.596	9.78
NKA	Auto-break	2003–2010	– (ns)	0.213	9.96
		2011–2015	– (ns)	0.723	12.53
		2016–2022	+ (*)	0.684	10.72
	Adjusted	2003–2008	– (*)	0.811	8.31
		2009–2014	– (ns)	0.087	13.31
		2015–2022	+ (*)	0.622	10.27

Note: Auto-break indicates the segmentation scheme based on the minimum SSE criterion, and Adjusted indicates the segmentation scheme used for subsequent analyses. Trend indicates the trend direction and significance, where + and – denote increasing and decreasing trends, respectively, and ns, *, and ** denote $p \geq 0.05$, $p < 0.05$, and $p < 0.01$, respectively. WSA, KA, and NKA denote the whole study area, karst area, and non-karst area, respectively.

3.2. PUE Chain Decomposition: Relative Contributions of Components and Interaction Terms

Variance decomposition of the PUE chain for 2003–2022 showed that SM/PRE, together with its interactions with other components, made the largest relative contribution to PUE variability (Figure 5). Across the whole study area, independent components accounted for 54.55% of the total relative contribution, while interaction terms accounted for 45.45%. Thus, temporal variation in PUE was associated not only with changes in individual chain components but also with covariation among components. SM/PRE alone contributed 33.33%, roughly four to five times that of GPP/T (6.23%), T/ET (7.53%), or ET/SM (7.46%). Among interaction terms, GPP/T $\cap$ ET/SM and T/ET $\cap$ SM/PRE ranked highest at 9.33% and 9.03%, followed by GPP/T $\cap$ SM/PRE (8.18%) and ET/SM $\cap$ SM/PRE (7.73%). All terms involving SM/PRE together contributed 58.27%, indicating that PUE variability in the four-component decomposition was mainly concentrated around the SM/PRE-related diagnostic terms.

In both karst and non-karst areas, SM/PRE was the largest independent component, contributing 34.00% and 32.82%, respectively. Independent components accounted for 55.74% of the total contribution in karst areas and 53.64% in non-karst areas, whereas interaction terms accounted for 44.26% and 46.36%, respectively. Among the interaction

terms involving SM/PRE, the relative contributions of $GPP/T \cap SM/PRE$, $T/ET \cap SM/PRE$, and $ET/SM \cap SM/PRE$ were 7.46%, 8.65%, and 7.46% in karst areas and 8.73%, 9.32%, and 7.94% in non-karst areas, respectively.

The contribution structure shifted notably across the three temporal phases (Figure 5). During 2003–2008, SM/PRE remained the largest single contributor (33.21%), with $T/ET \cap SM/PRE$ (10.99%), $GPP/T \cap ET/SM$ (9.62%), and $ET/SM \cap SM/PRE$ (9.50%) as the leading interaction terms. During 2009–2014, interaction terms accounted for 51.47% of the total contribution, exceeding the 48.53% contributed by independent components. SM/PRE remained the largest single term, with a contribution of 31.62%. The interaction terms $ET/SM \cap SM/PRE$ and $T/ET \cap SM/PRE$ also increased, reaching 12.53% and 12.49%, respectively. During 2015–2022, the independent contribution of SM/PRE increased to 35.09%, the highest value among the three phases. $T/ET \cap SM/PRE$ remained at 11.86%, whereas $ET/SM \cap SM/PRE$ decreased to 7.03%. Overall, SM/PRE was the leading contributor in all three phases, while interaction terms were most important during 2009–2014.

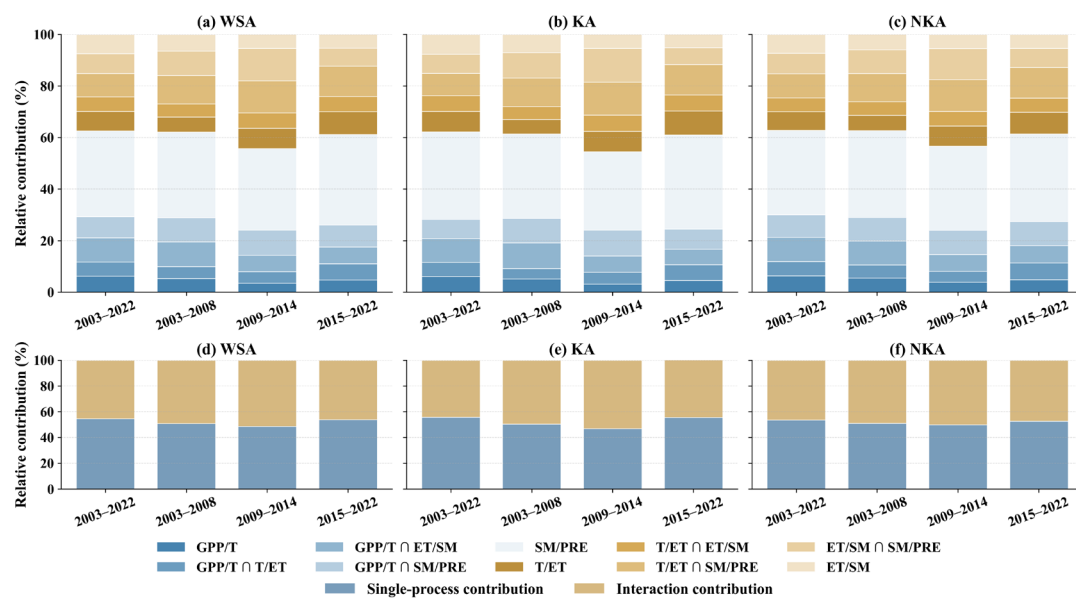


Figure 5. Relative contributions of PUE chain components and their interaction terms to PUE variance during 2003–2022 and across different sub-periods. (a–c) Relative contributions of individual chain components and interaction terms in the whole study area (WSA), karst area (KA), and non-karst area (NKA), respectively. (d–f) Comparison between the total contribution of individual chain components and that of interaction terms in WSA, KA, and NKA, respectively.

Spatially, the relative contributions of the chain components and interaction terms varied across the study area during 2003–2022 (Figure 6). Independent and interaction contributions showed different spatial patterns, suggesting that the dominant sources of PUE variability were not the same everywhere. High SM/PRE contributions were mainly found in the central study area and southern Guangxi. High T/ET contributions occurred in northwestern Yunnan and northwestern Guizhou, while high ET/SM contributions were concentrated in central–southern Guangxi. Among the interaction terms, $GPP/T \cap SM/PRE$ had higher values in southwestern Yunnan, $T/ET \cap SM/PRE$ was more evident in the eastern part of the study area, and $ET/SM \cap SM/PRE$ was lower in southern Guangxi and western Guizhou.

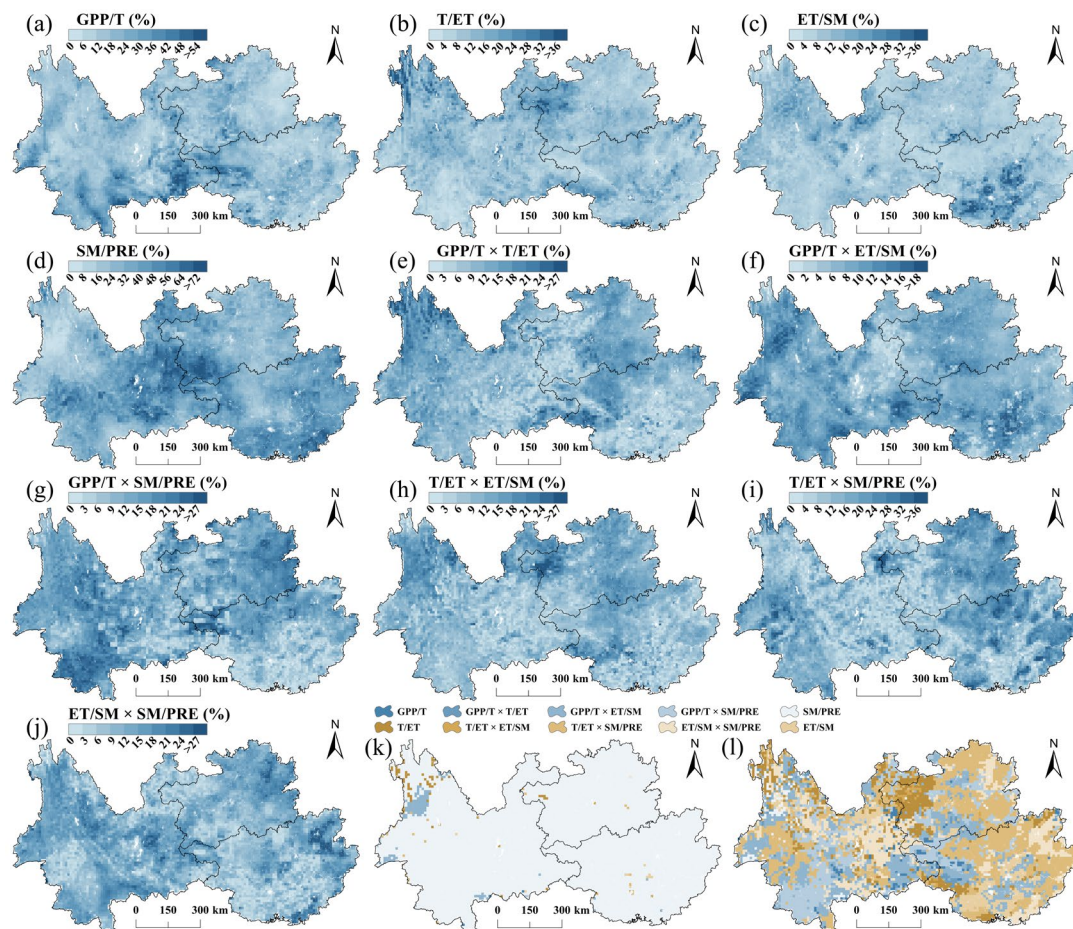


Figure 6. Spatial distributions of relative contributions of PUE chain components and their interaction terms to PUE variance during 2003–2022. (a–d) Relative contributions of individual chain components. (e–j) Relative contributions of pairwise interaction terms. (k,l) Spatial distributions of the first and second dominant contributors, respectively.

The dominant-term maps further showed that the leading contributor was spatially consistent (Figure 6k,l). SM/PRE ranked first across 96.77% of the study area. The second-ranked contributor, by contrast, showed stronger spatial heterogeneity: T/ET∩SM/PRE was most frequent (29.11%), followed by GPP/T∩ET/SM (17.94%), GPP/T∩SM/PRE (15.79%), and ET/SM∩SM/PRE (14.08%). Overall, SM/PRE was the main contributor to PUE variability, while its interaction terms explained additional regional and phase-specific differences.

3.3. Environmental Drivers of PUE Chain Components

3.3.1. Model Performance Evaluation

Figure 7 shows the prediction performance for each chain component under the four landform and drought–humid scenario combinations. Model performance differed across both scenarios and components. Across the 16 modeling cases, no single algorithm was the best in every case, indicating that the environmental responses of the chain components varied by scenario.



Figure 7. Model performance for the four PUE chain components under different landform types and drought–humid scenarios. Columns show the four scenarios: K-Drought, K-Humid, NK-Drought, and NK-Humid. Rows show the three performance metrics: R^2 , RMSE, and MAE. Within each panel, the horizontal axis shows the chain components, and the vertical axis shows the six models. Cell values give the model performance, and colors show the relative performance among models for the same chain component.

Among the individual models, CatBoost ranked first most often, giving the best performance in 11 of the 16 cases. Under the K-Drought scenario, CatBoost had the highest accuracy for all four components, GPP/T, T/ET, ET/SM, and SM/PRE, with R^2 values of 0.905, 0.837, 0.886, and 0.924, respectively. Under K-Humid, CatBoost performed best for T/ET, ET/SM, and SM/PRE, with R^2 values of 0.796, 0.894, and 0.936, respectively. XGBoost gave the best individual-model result for GPP/T ($R^2 = 0.896$). Under NK-Drought, CatBoost ranked first for GPP/T and T/ET ($R^2 = 0.920$ and 0.915), while GBRT performed best for ET/SM ($R^2 = 0.871$) and XGBoost for SM/PRE ($R^2 = 0.927$). Under NK-Humid, CatBoost again ranked first for GPP/T and T/ET ($R^2 = 0.899$ and 0.889), whereas XGBoost performed best for ET/SM and SM/PRE. These results show that the best individual model depended on the landform type, drought–humid condition, and chain component.

By comparison, the Stacking model exhibited greater consistency and stability across scenarios. It achieved the highest R^2 in 15 of the 16 cases, with MAE and RMSE generally at the lowest levels. The only exception was ET/SM under K-Humid, where CatBoost achieved a marginally higher R^2 (0.894) than Stacking (0.892). In terms of the mean R^2 across the four chain components, the NK-Drought, NK-Humid, K-Drought, and K-Humid scenarios yielded values of 0.911, 0.905, 0.891, and 0.883, respectively, indicating slightly better overall performance in non-karst areas than in karst areas. Although individual models attained high accuracy in specific scenario–component combinations, Stacking outperformed them in most cases. In addition, residual spatial autocorrelation analysis showed low Moran’s I values and high effective sample size ratios across the 16 scenario–component combinations, indicating that residual spatial dependence after accounting for the environmental predictors was weak (Supplementary Note S3). Subsequent driver identification and SHAP-based interpretability analyses were therefore conducted using the Stacking model.

3.3.2. Relative Importance of Environmental Factors

To reveal the differentiated driving effects of environmental factors on PUE chain components under drought and humid conditions in both karst and non-karst areas, and SHAP was applied to quantify the relative importance of each environmental factor (Figure 8). Across the four chain components, the leading factors were relatively stable under different scenarios, but the top three factor combinations and their importance shares differed notably.

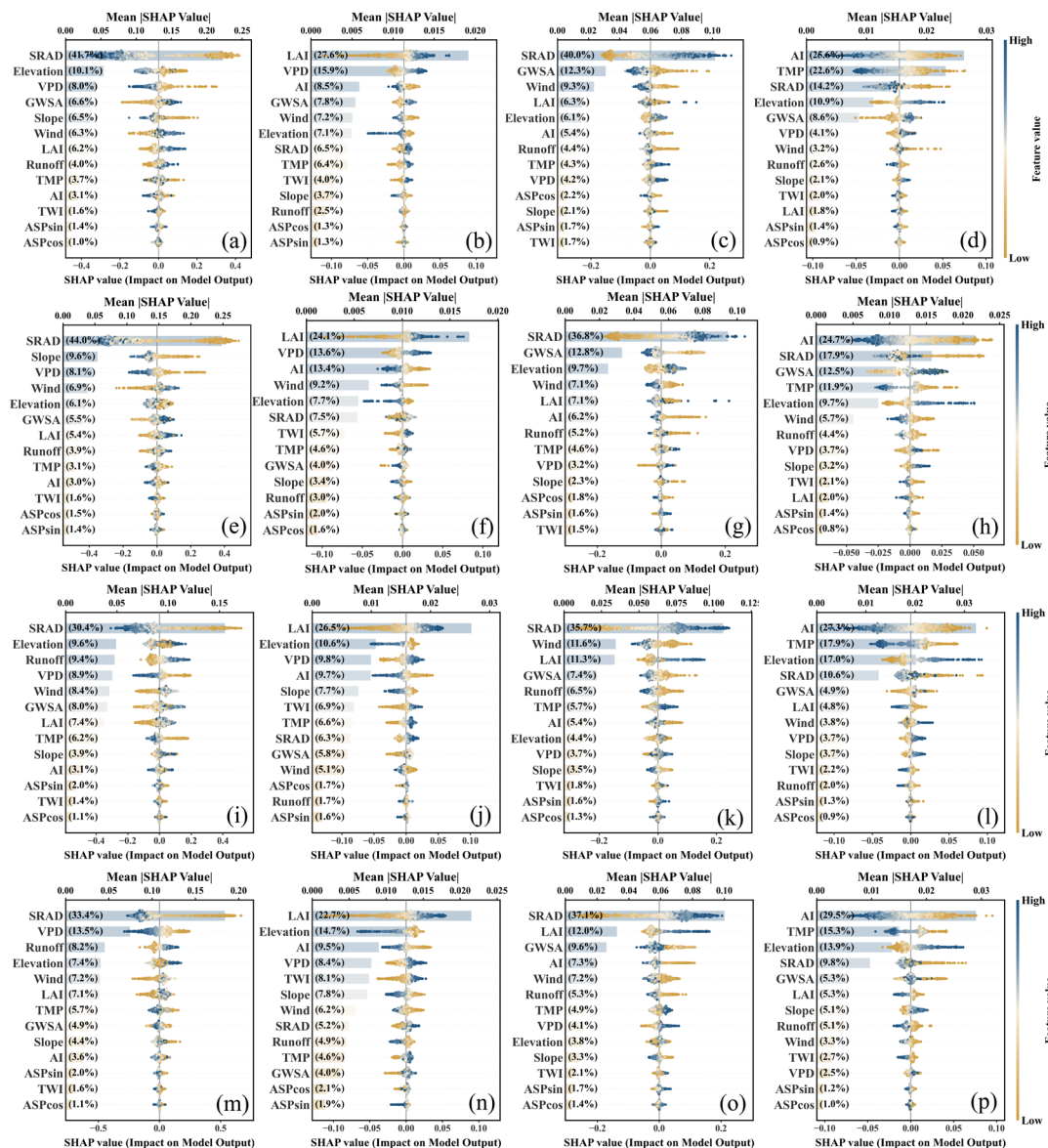


Figure 8. SHAP summary plots for each PUE chain component under different geomorphological types and drought-humid scenarios. Panels (a–d), (e–h), (i–l), and (m–p) correspond to the K-Drought, K-Humid, NK-Drought, and NK-Humid scenarios, respectively, with GPP/T, T/ET, ET/SM, and SM/PRE shown in sequence within each group.

For GPP/T, SRAD was the top-ranked factor in all four scenarios, with importance shares of 30.44–44.03%. The top three factor combinations were SRAD–Elevation–VPD, SRAD–Slope–VPD, SRAD–Elevation–Runoff, and SRAD–VPD–Runoff under K-Drought, K-Humid, NK-Drought, and NK-Humid, with cumulative shares of 59.74%, 61.75%, 49.47%, and 55.04%; the cumulative shares in karst areas were generally higher than those in non-karst areas. The SHAP summary plot showed that increases in SRAD and VPD

tended to reduce GPP/T SHAP values. For T/ET, LAI ranked first in all scenarios, with importance shares of 22.65–27.63%. The top three combinations in both karst scenarios were LAI–VPD–AI, while those in non-karst areas were LAI–Elevation–VPD and LAI–Elevation–AI, with cumulative shares of 52.05%, 51.13%, 46.84%, and 46.81%, indicating that high-importance factors were more concentrated in karst areas. The SHAP summary plot showed that increases in LAI and VPD generally raised T/ET predictions, whereas increases in AI and Elevation tended to lower them.

For ET/SM, SRAD was likewise the dominant factor across all four scenarios, with importance shares of 35.73–39.98%. The top three combinations were SRAD–GWSA–Wind, SRAD–GWSA–Elevation, SRAD–Wind–LAI, and SRAD–LAI–GWSA, with cumulative shares ranging from 58.69% to 61.51%—relatively similar across scenarios. Increases in SRAD and LAI generally raised ET/SM predictions, while increases in GWSA and Run-off tended to lower them. SM/PRE, by contrast, was dominated by AI, with importance shares of 24.71–29.49%. The cumulative shares of the top three factors ranged from 55.14% to 62.45%, and were generally higher under drought scenarios than under humid scenarios. The corresponding top three combinations were AI–TMP–SRAD, AI–SRAD–GWSA, AI–TMP–Elevation, and AI–TMP–Elevation. Increases in AI and TMP generally reduced SM/PRE predictions; in karst areas, increasing GWSA tended to raise SM/PRE predictions, whereas its directional effect was less clear in non-karst areas. Overall, the high-importance factor compositions of GPP/T and ET/SM were relatively stable, while T/ET and SM/PRE exhibited more pronounced scenario-specific differences.

3.3.3. SHAP Dependence Relationships of Dominant Factors

To further compare the response differences in dominant factors across scenarios, SHAP dependence plots of the leading factors were generated for the four PUE chain components under K-Drought, K-Humid, NK-Drought, and NK-Humid scenarios (Figure 9). A SHAP value above zero indicates that an increase in the factor value raises the model prediction of the corresponding component, a value below zero indicates a reduction, and the position where SHAP equals zero approximates the threshold at which the influence direction reverses. Across the four components, the dominant factors showed similar response directions among scenarios, but their threshold positions differed.

For GPP/T, SHAP values generally decreased as SRAD increased, changing from positive to negative effects. The SHAP = 0 thresholds were approximately 1270.09, 1221.30, 1330.23, and 1269.22 under K-Drought, K-Humid, NK-Drought, and NK-Humid, respectively. Thresholds were higher under drought than under humid conditions, and higher in non-karst areas than in karst areas. For T/ET, SHAP values increased with LAI, changing from negative to positive effects. The thresholds were approximately 2.28, 2.46, 2.79, and 2.96. Non-karst areas had higher thresholds than karst areas, and humid scenarios had higher thresholds than drought scenarios.

For ET/SM, SHAP values increased with SRAD. Thresholds were approximately 1285.70, 1235.47, 1335.77, and 1281.76 under K-Drought, K-Humid, NK-Drought, and NK-Humid—a scenario pattern resembling that of GPP/T, with drought-scenario thresholds higher than humid-scenario thresholds and non-karst thresholds higher than karst thresholds. For SM/PRE, SHAP values declined with increasing AI, with thresholds of approximately 1.42, 1.92, 1.42, and 1.86. Under drought scenarios, karst and non-karst thresholds were identical, while under humid scenarios the karst threshold was slightly higher than the non-karst threshold. In general, the response directions of the dominant factors remained stable across scenarios, but the thresholds at which influence directions reversed were jointly modulated by the landform type and drought–humid condition.

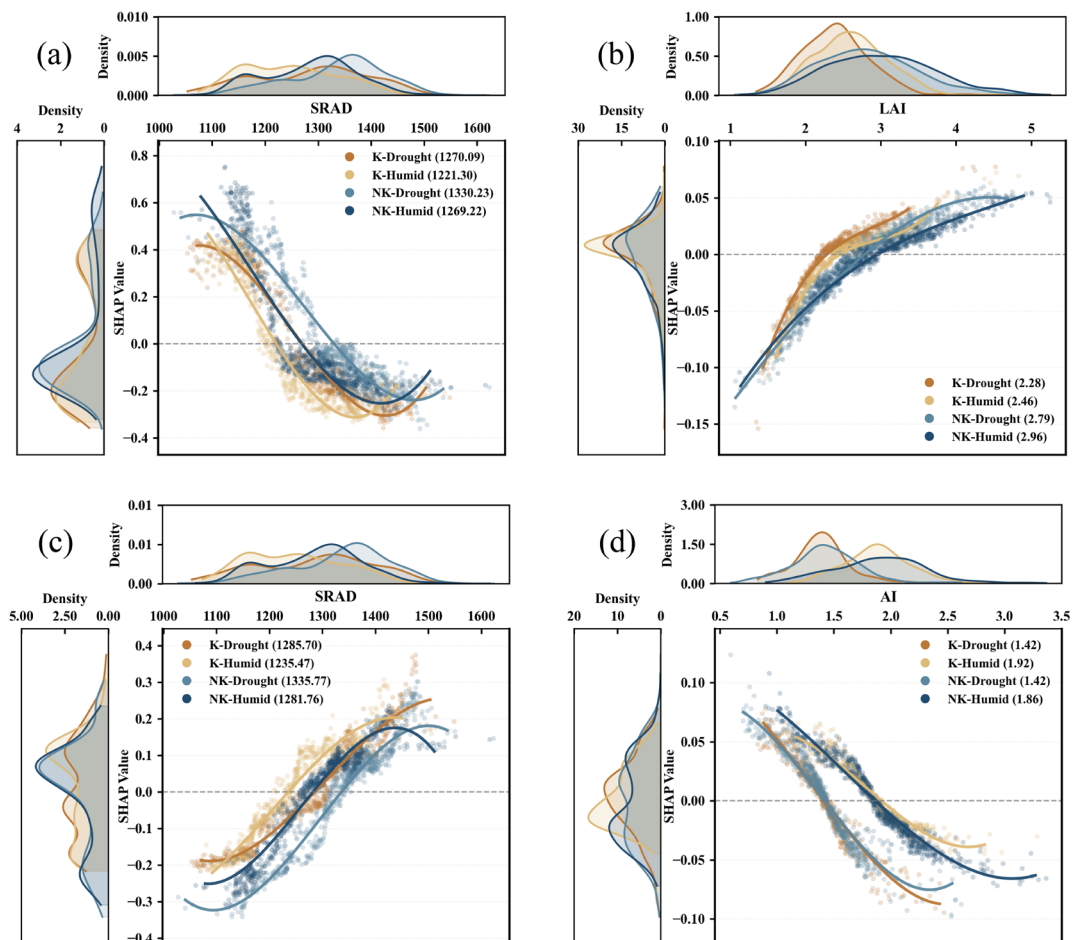


Figure 9. SHAP dependence plots for the dominant driving factors of each PUE chain component under different geomorphological types and drought–humid scenarios. (a–d) show the SHAP response relationships for GPP/T–SRAD, T/ET–LAI, ET/SM–SRAD, and SM/PRE–AI under K-Drought, K-Humid, NK-Drought, and NK-Humid scenarios, respectively.

4. Discussion

4.1. Process-Chain Diagnosis of Carbon–Water Coupling in Vulnerable Land Ecosystems

Water-use efficiency describes how terrestrial ecosystems couple carbon gain with water use. Previous studies have commonly used WUE, SWUE, and PUE to summarize the overall relationship between vegetation productivity and a particular water-related variable. These indices, however, say little about what happens after rainfall enters the soil, or how soil water retention, evapotranspiration output, and transpiration partitioning jointly support carbon fixation through a sequence of ecohydrological steps [8–10]. By developing a chain decomposition framework, this study shifts the analysis of precipitation use efficiency from differences in the endpoint ratio to the identification of constraints within the intermediate stages.

The results in Section 3.2 show that the spatial and temporal variation in PUE was associated with the combined variation in several chain components and their interaction terms. A direct comparison between GPP and precipitation alone therefore makes it difficult to identify which intermediate terms are most closely related to changes in carbon–water coupling. This limitation is especially relevant in karst regions, which are vulnerable land ecosystems characterized by thin soils, complex water transport pathways, and strong surface–subsurface hydrological coupling [18,19]. In addition, the regional comparison in Section 3.1 showed significant differences in PUE and all four chain components between karst and non-karst areas. The log-ratio mean decomposition further indi-

cated that the higher mean PUE in non-karst areas was mainly associated with positive differences in ET/SM and T/ET, especially ET/SM, whereas GPP/T and SM/PRE partly offset this difference (Table S3). The chain framework used here therefore helps link regional PUE differences with the diagnostic terms and interaction structures that contribute to PUE variability. In doing so, it provides a more structured diagnostic interpretation of carbon–water coupling and offers a practical basis for identifying potential water-use limitation stages and informing regional soil and water management.

4.2. Dominant Ecohydrological Signals Revealed by Chain Decomposition

The variance–covariance decomposition identified SM/PRE as the largest contributor to the temporal variability of vegetation precipitation use efficiency in Southwest China. Additional log-space, signed, and five-factor decompositions confirmed that this result was not sensitive to the Taylor approximation. They further showed that the large contribution of SM/PRE was mainly associated with the sensitivity of PUE to PRE variation (Supplementary Note S1). Therefore, within the chain framework used here, SM/PRE should be interpreted as a diagnostic ratio describing soil moisture status relative to precipitation input, rather than as direct physical evidence of precipitation-to-soil-water or root-zone-water conversion. Verifying the actual links among precipitation, soil water, and vegetation water use would require more direct hydrological evidence, such as stable isotope observations across different soil layers [62]. Such information was beyond the scope of the present remote-sensing-based decomposition. Previous studies have shown that soil moisture and antecedent moisture conditions are closely related to vegetation water stress and drought propagation [63,64]. Thus, the large contribution of SM/PRE-related terms indicates that temporal changes in PUE were closely associated with precipitation sensitivity and soil moisture status relative to precipitation input. Evapotranspiration output, transpiration partitioning, and transpiration-based carbon fixation further shaped the final PUE variation.

The phase analysis provides a temporal perspective on this interpretation. By combining breakpoint detection with drought-index information, we found that interaction terms contributed more than independent terms during 2009–2014, when PUE fluctuated strongly and drought conditions were more severe. During 2015–2022, when PUE gradually recovered, the independent contribution of SM/PRE increased markedly. This pattern suggests that chain components were more tightly coupled during periods of stronger climatic fluctuation. In contrast, the later recovery of PUE was more closely associated with variation in the SM/PRE-related diagnostic term.

The SHAP results further clarified which environmental signals were associated with different parts of the chain. GPP/T and ET/SM were both mainly associated with SRAD, but their response directions differed. Higher SRAD was associated with higher ET/SM but lower GPP/T, suggesting that radiation-related energy supply and atmospheric demand may affect evapotranspiration output and carbon gain per unit transpiration in different ways [3,65]. T/ET was mainly related to LAI, consistent with the role of canopy structure in regulating the transpiration fraction [17]. SM/PRE was most strongly related to the aridity index, suggesting that background water balance is an important external condition shaping soil moisture status relative to precipitation input [10].

The threshold results showed broadly similar response directions but clear differences in threshold positions between drought and humid scenarios. Under drought conditions, the SRAD thresholds for GPP/T and ET/SM were generally higher than those under humid conditions. This suggests that, when water is limited, the response of radiation-related effects may shift only at higher radiation levels. Previous studies have also shown that stronger radiation during drought is often accompanied by higher evaporative demand and greater moisture-deficit pressure, which do not necessarily increase carbon fix-

ation and evapotranspiration output simultaneously [65–68]. The LAI threshold for T/ET was generally higher under humid conditions, implying that a larger transpiration fraction may require more developed canopy cover when water is relatively sufficient [69–71]. In contrast, the AI threshold for SM/PRE was lower under drought conditions, indicating that the early diagnostic stage of the PUE chain is more sensitive to background water-balance changes under water-limited conditions [64,68,72,73].

4.3. Diagnostic Differences Between Karst and Non-Karst Areas

Differences along the PUE chain between karst and non-karst areas suggest that the main diagnostic stages associated with PUE variation differed between the two landform types. Karst areas showed relatively higher GPP/T and SM/PRE, whereas non-karst areas showed relatively higher T/ET and ET/SM, with overall PUE being higher in non-karst areas. This suggests that the relative advantages of karst areas in soil moisture status and transpiration-based carbon fixation did not necessarily translate into higher overall PUE. In contrast, the higher T/ET and ET/SM in non-karst areas were important diagnostic terms associated with their higher PUE. The PUE difference between the two landform types was therefore more likely related to the combined variation in multiple chain components rather than to a single efficiency term.

This contrast may be linked to stronger subsurface or near-surface water-storage signals in karst areas. The SHAP results showed that GWSA ranked among the top three important factors for ET/SM in karst areas under both drought and humid scenarios. In non-karst areas, however, GWSA entered the top three only in selected scenarios and at lower ranks. In karst areas, thin soils, permeable bedrock, and well-developed fracture systems form a dual surface–subsurface hydrological structure, which may make the upstream and intermediate stages of the PUE chain more closely associated with subsurface or near-surface water-storage conditions [18,20,74–76]. It should also be noted that the SM data used in this study represent an integrated value over the 0–1 m depth range. In karst areas, this signal may partly include shallow fracture water or epikarst storage information [20,74]. Therefore, the combination of slightly higher SM and lower ET/SM in karst areas suggests that higher water-storage signals do not necessarily correspond to higher evapotranspiration output relative to the soil moisture pool.

Response thresholds derived from SHAP dependence relationships further suggest that some chain components in karst areas may be more sensitive to environmental variation. Under the same drought–humid conditions, the SRAD thresholds for GPP/T and ET/SM, as well as the LAI threshold for T/ET, were lower in karst areas than in non-karst areas. This indicates that model-inferred response transitions occurred at lower predictor values in karst areas when radiation conditions strengthened or canopy structure changed. These thresholds should be understood as apparent transition points inferred from the model, rather than as strict physical thresholds. Nevertheless, their systematic differences between the two landform types suggest that the intermediate diagnostic stages in karst areas may respond more sensitively to environmental fluctuations [21,72].

The dominant factor combinations also differed between the two landform types. In karst areas, the high-importance factors for T/ET were mainly represented by the LAI–VPD–AI combination, suggesting that transpiration partitioning was jointly associated with canopy structure, atmospheric dryness, and background water balance. In non-karst areas, the LAI–Elevation combination was more prominent, indicating a stronger association with vegetation structure and topographic setting. Overall, karst areas showed more prominent subsurface or near-surface water-storage signals and more sensitive model-inferred response thresholds, whereas non-karst areas showed diagnostic patterns more closely related to near-surface hydrothermal conditions and topographic setting.

4.4. Implications for Vulnerable Land Ecosystems and Sustainable Land Management

These results help explain why vulnerable land ecosystems may respond differently under changing hydroclimatic conditions. In Southwest China, karst landscapes are characterized by thin soils, strong surface–subsurface hydrological connectivity, and uneven water-storage conditions. These features make vegetation productivity sensitive to changes in water availability [18,20]. The chain decomposition results showed that PUE variation was mainly concentrated around SM/PRE-related diagnostic terms and their interactions with other chain components. This suggests that carbon–water coupling in this region is not determined only by transpiration-based carbon fixation or evapotranspiration partitioning. It is also closely associated with the soil moisture condition maintained relative to precipitation input, although this ratio should not be interpreted as a direct measure of precipitation conversion into plant-available water.

This point is particularly relevant to karst landscapes, where high precipitation does not always translate into effective ecological water supply [18,74]. The stronger GWSA-related signal and lower model-inferred response thresholds in karst areas suggest that vegetation–water relationships may respond more sensitively to changes in radiation, canopy structure, aridity background, and subsurface water conditions. Ecological restoration in karst regions should therefore not focus only on increasing vegetation cover or productivity. Because vegetation dynamics can also modify soil moisture and runoff processes [77], soil moisture retention, subsurface water conditions, vegetation water demand, and the possible mismatch between water-storage signals and effective water output should be considered together.

For land management, the process-chain perspective can help identify the stages where potential water-use limitations may occur along the pathway from precipitation input to carbon fixation. Where SM/PRE-related diagnostic terms make a large contribution, measures that conserve soil water, reduce rapid runoff and leakage where feasible, and maintain vegetation structures suited to local water availability may be more useful than approaches aimed only at increasing biomass [18,24]. More broadly, this perspective has important implications for water-resource management under changing land-use conditions [78–80]. In non-karst areas, higher PUE was more closely associated with transpiration partitioning and evapotranspiration output. Vegetation structure and near-surface hydrothermal conditions may therefore require more attention. Management strategies should differ between karst and non-karst landscapes according to the main diagnostic stages associated with PUE variation.

The framework may also be useful for assessing vegetation–hydrology–climate responses in other vulnerable land ecosystems. By linking precipitation input, soil moisture status, evapotranspiration output, transpiration partitioning, and carbon fixation, it moves the analysis beyond terminal efficiency ratios. More importantly, it helps identify intermediate diagnostic stages where water-use limitations may emerge. This can support ecological restoration planning, drought adaptation, and sustainable management in heterogeneous land systems exposed to climate variability and global change.

4.5. Limitations and Future Directions

Several limitations remain in this study. First, the growing-season annual data used here can capture interannual variation and spatial patterns in PUE, but they cannot resolve short-term ecohydrological responses. Second, although we selected data products that have shown good performance in similar regions and applied consistent preprocessing, retrieval errors and scale mismatches remain unavoidable in multi-source datasets [45,81]. The magnitudes of the decomposition terms may also change if alternative GPP, ET, T, SM, PRE, or groundwater products are used. In addition, pixel-level accuracy, Kappa, and confusion-matrix validation were unavailable for the karst/non-karst map,

which may add uncertainty near lithological boundaries or mixed grid cells. Third, the chain decomposition framework can identify where PUE variability is mainly concentrated along the sequence of precipitation input, soil moisture status, evapotranspiration output, transpiration partitioning, and carbon fixation. However, it does not explicitly simulate hydrological processes such as runoff generation, infiltration, drainage, groundwater flow, or water-transfer pathways.

The Stacking model and SHAP analysis used in this study were useful for identifying important predictors and nonlinear response patterns. The use of Stacking also reduced the dependence on any single machine learning algorithm. Nevertheless, the attribution results should be interpreted as model-based statistical contributions and associations among the variables included in the analysis. They do not establish causal relationships in a strict sense. Although residual spatial autocorrelation was assessed, spatial blocking cross-validation was not performed; therefore, the ML-SHAP results should be interpreted as explanatory associations within the study region rather than spatially transferable predictions.

Future work could examine PUE and its intermediate components at within-year time scales, where short-term hydrological responses and seasonal vegetation adjustments can be better identified. Field observations, such as layered soil moisture measurements, groundwater-level monitoring, and isotope-based water-source tracing, would help constrain the physical meaning and uncertainty of key diagnostic terms [62]. Another useful step would be to combine the chain decomposition framework with process-oriented hydrological models and causal-inference approaches [82,83]. Such approaches could provide useful guidance for incorporating more explicit constraints on runoff generation, infiltration, drainage, and groundwater flow into future PUE chain diagnosis. They would also help test and refine the interpretation of how different ecohydrological stages are associated with carbon–water coupling in terrestrial ecosystems. Such work could provide stronger support for ecological restoration, agricultural water management, and adaptation planning in vulnerable land ecosystems under climate change.

5. Conclusions

This study developed a PUE chain decomposition framework ($PUE = GPP/T \times T/ET \times ET/SM \times SM/PRE$) and combined variance decomposition, Stacking ensemble learning, and SHAP analysis to diagnose the chain components and environmental associations of PUE variability across karst and non-karst landscapes in Southwest China. The main conclusions are as follows:

- (1) PUE and its chain components exhibited pronounced spatiotemporal heterogeneity. Spatially, PUE was generally higher in non-karst areas than in karst areas, with significant differences in all chain components between the two landform types. Temporally, PUE followed a three-phase trajectory, characterized by an initial decline, intensified fluctuations during the middle period, and recovery growth in the later period.
- (2) Variance decomposition identified SM/PRE and its associated interaction terms as major contributors to PUE variability, mainly reflecting the sensitivity of PUE to precipitation variation and soil moisture status relative to precipitation input. Phase-specific changes in PUE were accompanied by shifts between independent chain-term contributions and interaction contributions, suggesting that the diagnostic structure of PUE varied with hydroclimatic background.
- (3) Differences in PUE between karst and non-karst landscapes were associated with the combined variation in multiple chain components rather than a single efficiency term. Karst landscapes showed relatively higher GPP/T and SM/PRE, whereas non-karst landscapes showed relatively higher T/ET and ET/SM. The SHAP results fur-

ther indicated stronger GWSA-related signals and lower model-inferred response thresholds in karst areas, while non-karst areas were more closely associated with near-surface hydrothermal conditions and topographic setting.

- (4) Different chain components were associated with distinct environmental signals. GPP/T and ET/SM were both mainly associated with solar radiation but showed opposite response directions. T/ET was mainly associated with leaf area index, whereas SM/PRE was primarily associated with the regional moisture background. The response thresholds of dominant factors differed between landform types and drought–humid conditions, indicating that the environmental sensitivity of PUE chain components varied across scenarios.
- (5) Future studies should apply the chain decomposition framework at finer temporal scales and integrate field observations, process-oriented hydrological models, and causal-inference approaches. These efforts would help constrain the physical meaning of key diagnostic terms and refine the interpretation of carbon–water coupling in vulnerable land ecosystems.

Overall, this study shows that the PUE chain decomposition framework can help identify the diagnostic stages and environmental associations underlying PUE variability across contrasting landforms. The framework provides a useful basis for assessing carbon–water coupling in vulnerable land ecosystems and for informing ecological restoration and sustainable land management under changing hydroclimatic conditions.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/land15071243/s1>, Supplementary Note S1. Log-Space and Five-Factor Decomposition. Table S1. Four-factor log-space variance decomposition for the full study area during 2003–2022. Table S2. Five-factor log-space variance decomposition for the full study area during 2003–2022. Table S3. Log-ratio decomposition of the PUE difference between non-karst and karst areas. Table S4. Effective sample size estimates after spatial autocorrelation correction. Supplementary Note S2. Log-Ratio Decomposition of the PUE Difference between Karst and Non-Karst Areas. Supplementary Note S3. Residual Spatial Autocorrelation and Effective Sample Size.

Author Contributions: Conceptualization, Y.H. and S.L.; methodology, Y.H. and S.Q.; software, Y.H.; validation, Y.H. and S.L.; formal analysis, Y.H.; investigation, Y.H. and M.L.; resources, S.L.; data curation, Y.H. and S.L.; writing—original draft preparation, Y.H.; writing—review and editing, Y.H., S.L., S.Q. and M.L.; visualization, Y.H.; supervision, S.L.; project administration, S.L.; funding acquisition, S.L. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the National Natural Science Foundation of China, grant number 42161029.

Data Availability Statement: The original contributions presented in this study are included in the article/Supplementary Material. Further inquiries can be directed to the corresponding authors.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

AI	Aridity index
ASPCos	Cosine-transformed aspect
ASPSin	Sine-transformed aspect
CV	Coefficient of variation
ET	Evapotranspiration
GPP	Gross primary productivity

GWSA	Groundwater storage anomaly
KA	Karst area
K-Drought	Karst drought scenario
K-Humid	Karst humid scenario
NKA	Non-karst area
NK-Drought	Non-karst drought scenario
NK-Humid	Non-karst humid scenario
LAI	Leaf area index
MAE	Mean absolute error
PET	Potential evapotranspiration
PRE	Precipitation
PUE	Precipitation use efficiency
RC	Relative contribution
RF	Random forest
RMSE	Root mean square error
SHAP	Shapley additive explanations
SM	Soil moisture
SPEI	Standardized Precipitation Evapotranspiration Index
SRAD	Surface solar radiation downwards
SSE	Sum of squared errors
SWUE	Soil water-use efficiency
T	Transpiration
TMP	Temperature
TWI	Topographic wetness index
VPD	Vapor pressure deficit
WSA	Whole study area
WUE	Water use efficiency

References

1. Gentine, P.; Green, J.K.; Guérin, M.; Humphrey, V.; Seneviratne, S.I.; Zhang, Y.; Zhou, S. Coupling between the Terrestrial Carbon and Water Cycles—A Review. *Environ. Res. Lett.* **2019**, *14*, 83003. <https://doi.org/10.1088/1748-9326/ab22d6>.
2. Liu, X.; Feng, X.; Fu, B. Changes in Global Terrestrial Ecosystem Water Use Efficiency Are Closely Related to Soil Moisture. *Sci. Total Environ.* **2020**, *698*, 134165. <https://doi.org/10.1016/j.scitotenv.2019.134165>.
3. Li, F.; Xiao, J.; Chen, J.; Ballantyne, A.; Jin, K.; Li, B.; Abraha, M.; John, R. Global Water Use Efficiency Saturation Due to Increased Vapor Pressure Deficit. *Science* **2023**, *381*, 672–677. <https://doi.org/10.1126/science.adf5041>.
4. Zhu, Z.; Piao, S.; Myneni, R.B.; Huang, M.; Zeng, Z.; Canadell, J.G.; Ciais, P.; Sitch, S.; Friedlingstein, P.; Arneeth, A.; et al. Greening of the Earth and Its Drivers. *Nat. Clim. Change* **2016**, *6*, 791–795. <https://doi.org/10.1038/nclimate3004>.
5. Zeng, Z.; Piao, S.; Li, L.Z.X.; Wang, T.; Ciais, P.; Lian, X.; Yang, Y.; Mao, J.; Shi, X.; Myneni, R.B. Impact of Earth Greening on the Terrestrial Water Cycle. *J. Clim.* **2018**, *31*, 2633–2650. <https://doi.org/10.1175/JCLI-D-17-0236.1>.
6. Hu, Z.Y.; Dai, Q.H.; Yan, Y.J.; Zhang, Y.; Li, H.Y.; Zhou, H.; Yao, Y.W. Dissecting the Characteristics and Driver Factors on Global Water Use Efficiency Using GLASS Data Sets. *Earth's Future* **2024**, *12*, e2024EF004630. <https://doi.org/10.1029/2024EF004630>.
7. Huxman, T.E.; Smith, M.D.; Fay, P.A.; Knapp, A.K.; Shaw, M.R.; Loik, M.E.; Smith, S.D.; Tissue, D.T.; Zak, J.C.; Weltzin, J.F.; et al. Convergence across Biomes to a Common Rain-Use Efficiency. *Nature* **2004**, *429*, 651–654. <https://doi.org/10.1038/nature02561>.
8. Liu, X.; Lai, Q.; Yin, S.; Bao, Y.; Qing, S.; Bayarsaikhan, S.; Bu, L.; Mei, L.; Li, Z.; Niu, J.; et al. Exploring Grassland Ecosystem Water Use Efficiency Using Indicators of Precipitation and Soil Moisture across the Mongolian Plateau. *Ecol. Indic.* **2022**, *142*, 109207. <https://doi.org/10.1016/j.ecolind.2022.109207>.
9. Ding, H.; Yuan, Z.; Shi, X.; Yin, J.; Chen, F.; Shi, M.; Zhang, F. Soil Moisture Content-Based Analysis of Terrestrial Ecosystems in China: Water Use Efficiency of Vegetation Systems. *Ecol. Indic.* **2023**, *150*, 110271. <https://doi.org/10.1016/j.ecolind.2023.110271>.
10. Gong, E.; Zhang, J.; Bai, T.; Wang, Z.; Bai, H.; Wang, J. Spatiotemporal Dynamics and Influencing Factors of Precipitation and Soil Water Use Efficiency on the Chinese Loess Plateau. *J. Hydrol.* **2026**, *664*, 134600. <https://doi.org/10.1016/j.jhydrol.2025.134600>.
11. Rodriguez-Iturbe, I. Ecohydrology: A Hydrologic Perspective of Climate-Soil-Vegetation Dynamics. *Water Resour. Res.* **2000**, *36*, 3–9. <https://doi.org/10.1029/1999WR900210>.

12. Seneviratne, S.I.; Corti, T.; Davin, E.L.; Hirschi, M.; Jaeger, E.B.; Lehner, I.; Orlowsky, B.; Teuling, A.J. Investigating Soil Moisture–Climate Interactions in a Changing Climate: A Review. *Earth Sci. Rev.* **2010**, *99*, 125–161. <https://doi.org/10.1016/j.earsci-rev.2010.02.004>.
13. Jasechko, S.; Sharp, Z.D.; Gibson, J.J.; Birks, S.J.; Yi, Y.; Fawcett, P.J. Terrestrial Water Fluxes Dominated by Transpiration. *Nature* **2013**, *496*, 347–350. <https://doi.org/10.1038/nature11983>.
14. Good, S.P.; Noone, D.; Bowen, G. Hydrologic Connectivity Constrains Partitioning of Global Terrestrial Water Fluxes. *Science* **2015**, *349*, 175–177. <https://doi.org/10.1126/science.aaa5931>.
15. Hu, Z.; Yu, G.; Fu, Y.; Sun, X.; Li, Y.; Shi, P.; Wang, Y.; Zheng, Z. Effects of Vegetation Control on Ecosystem Water Use Efficiency within and among Four Grassland Ecosystems in China. *Glob. Change Biol.* **2008**, *14*, 1609–1619. <https://doi.org/10.1111/j.1365-2486.2008.01582.x>.
16. Wang, L.; Li, Y.; Zhang, X.; Chen, K.; Siddique, K.H.M. Soil Water Content and Vapor Pressure Deficit Affect Ecosystem Water Use Efficiency through Different Pathways. *J. Hydrol.* **2024**, *640*, 131732. <https://doi.org/10.1016/j.jhydrol.2024.131732>.
17. Cao, R.; Hu, Z.; Jiang, Z.; Yang, Y.; Zhao, W.; Wu, G.; Feng, X.; Chen, R.; Hao, G. Shifts in Ecosystem Water Use Efficiency on China’s Loess Plateau Caused by the Interaction of Climatic and Biotic Factors over 1985–2015. *Agric. For. Meteorol.* **2020**, *291*, 108100. <https://doi.org/10.1016/j.agrformet.2020.108100>.
18. Zhou, Q.; Luo, Y.; Shi, C.; Li, Y. Hydrological Effects of Vegetation Restoration in Karst Areas Research: Progress and Challenges. *Trans. Earth Environ. Sustain.* **2023**, *1*, 177–204. <https://doi.org/10.1177/2754124X231199565>.
19. Zheng, M.; Fu, J.; Jin, Y.; Ji, Y.; Dong, S.; Liu, B. Impact of Soil Moisture Depth Variation on Agricultural Drought Monitoring in Karst and Non-Karst Areas of Southwest China: A Case Study of Yunnan Province. *Catena* **2025**, *259*, 109392. <https://doi.org/10.1016/j.catena.2025.109392>.
20. Huang, Z.; Yeh, P.J.-F.; Pan, Y.; Jiao, J.J.; Gong, H.; Li, X.; Güntner, A.; Zhu, Y.; Zhang, C.; Zheng, L. Detection of Large-Scale Groundwater Storage Variability over the Karstic Regions in Southwest China. *J. Hydrol.* **2019**, *569*, 409–422. <https://doi.org/10.1016/j.jhydrol.2018.11.071>.
21. Wang, L.; Yue, Y.; Cui, J.; Liu, H.; Shi, L.; Liang, B.; Li, Q.; Wang, K. Precipitation Sensitivity of Vegetation Growth in Southern China Depends on Geological Settings. *J. Hydrol.* **2024**, *643*, 131916. <https://doi.org/10.1016/j.jhydrol.2024.131916>.
22. Peng, D.; Zhou, Q.; Tang, X.; Yan, W.; Chen, M. Changes in Soil Moisture Caused Solely by Vegetation Restoration in the Karst Region of Southwest China. *J. Hydrol.* **2022**, *613*, 128460. <https://doi.org/10.1016/j.jhydrol.2022.128460>.
23. Wang, M.; Ding, Z.; Wu, C.; Song, L.; Ma, M.; Yu, P.; Lu, B.; Tang, X. Divergent Responses of Ecosystem Water-Use Efficiency to Extreme Seasonal Droughts in Southwest China. *Sci. Total Environ.* **2021**, *760*, 143427. <https://doi.org/10.1016/j.scitotenv.2020.143427>.
24. Ding, Z.; Liu, Y.; Wang, L.; Chen, Y.; Yu, P.; Ma, M.; Tang, X. Effects and Implications of Ecological Restoration Projects on Ecosystem Water Use Efficiency in the Karst Region of Southwest China. *Ecol. Eng.* **2021**, *170*, 106356. <https://doi.org/10.1016/j.ecoleng.2021.106356>.
25. Liu, X.; Yu, S.; Yang, Z.; Dong, J.; Peng, J. The First Global Multi-Timescale Daily SPEI Dataset from 1982 to 2021. *Sci. Data* **2024**, *11*, 223. <https://doi.org/10.1038/s41597-024-03047-z>.
26. Zhang, Y.; Kong, D.; Gan, R.; Chiew, F.H.S.; McVicar, T.R.; Zhang, Q.; Yang, Y. Coupled Estimation of 500 m and 8-Day Resolution Global Evapotranspiration and Gross Primary Production in 2002–2017. *Remote Sens. Environ.* **2019**, *222*, 165–182. <https://doi.org/10.1016/j.rse.2018.12.031>.
27. Shi, X.; She, D.; Xia, J.; Liu, R.; Wang, T. The Intercomparison of Six 0.1°×0.1° Spatial Resolution Evapotranspiration Products across Mainland China. *J. Hydrol.* **2024**, *633*, 130949. <https://doi.org/10.1016/j.jhydrol.2024.130949>.
28. Li, Q.; Shi, G.; Shanguan, W.; Nourani, V.; Li, J.; Li, L.; Huang, F.; Zhang, Y.; Wang, C.; Wang, D.; et al. A 1 Km Daily Soil Moisture Dataset over China Using in Situ Measurement and Machine Learning. *Earth Syst. Sci. Data* **2022**, *14*, 5267–5286. <https://doi.org/10.5194/essd-14-5267-2022>.
29. Beck, H.E.; Wood, E.F.; Pan, M.; Fisher, C.K.; Miralles, D.G.; Van Dijk, A.I.J.M.; McVicar, T.R.; Adler, R.F. MSWEP V2 Global 3-Hourly 0.1° Precipitation: Methodology and Quantitative Assessment. *Bull. Am. Meteorol. Soc.* **2019**, *100*, 473–500. <https://doi.org/10.1175/BAMS-D-17-0138.1>.
30. Xu, Z.; Wu, Z.; He, H.; Wu, X.; Zhou, J.; Zhang, Y.; Guo, X. Evaluating the Accuracy of MSWEP V2.1 and Its Performance for Drought Monitoring over Mainland China. *Atmos. Res.* **2019**, *226*, 17–31. <https://doi.org/10.1016/j.atmosres.2019.04.008>.
31. Zhang, L.; Lan, P.; Qin, G.; Mello, C.R.; Boyer, E.W.; Luo, P.; Guo, L. Evaluation of Three Gridded Precipitation Products to Quantify Water Inputs over Complex Mountainous Terrain of Western China. *Remote Sens.* **2021**, *13*, 3795. <https://doi.org/10.3390/rs13193795>.

32. Mo, C.; Lei, X.; Mo, X.; Ruan, R.; Tang, G.; Li, L.; Sun, G.; Jiang, C. Comprehensive Evaluation and Comparison of Ten Precipitation Products in Terms of Accuracy and Stability over a Typical Mountain Basin, Southwest China. *Atmos. Res.* **2024**, *297*, 107116. <https://doi.org/10.1016/j.atmosres.2023.107116>.
33. Shangguan, W.; Li, Q.; Shi, G. *A 1 km daily soil moisture dataset over China based on in-situ measurement (2000–2022)*; National Tibetan Plateau/Third Pole Environment Data Center: Beijing, China, 2022. <https://doi.org/10.11888/Terre.tpd.272415>.
34. Muñoz-Sabater, J.; Dutra, E.; Agustí-Panareda, A.; Albergel, C.; Arduini, G.; Balsamo, G.; Boussetta, S.; Choulga, M.; Harrigan, S.; Hersbach, H.; et al. ERA5-Land: A State-of-the-Art Global Reanalysis Dataset for Land Applications. *Earth Syst. Sci. Data* **2021**, *13*, 4349–4383. <https://doi.org/10.5194/essd-13-4349-2021>.
35. Martens, B.; Miralles, D.G.; Lievens, H.; Van Der Schalie, R.; De Jeu, R.A.M.; Fernández-Prieto, D.; Beck, H.E.; Dorigo, W.A.; Verhoest, N.E.C. GLEAM v3: Satellite-Based Land Evaporation and Root-Zone Soil Moisture. *Geosci. Model Dev.* **2017**, *10*, 1903–1925. <https://doi.org/10.5194/gmd-10-1903-2017>.
36. Harrigan, S.; Zsoter, E.; Alfieri, L.; Prudhomme, C.; Salamon, P.; Wetterhall, F.; Barnard, C.; Cloke, H.; Pappenberger, F. GloFAS-ERA5 Operational Global River Discharge Reanalysis 1979–Present. *Earth Syst. Sci. Data* **2020**, *12*, 2043–2060. <https://doi.org/10.5194/essd-12-2043-2020>.
37. Zhang, G.; Xu, T.; Yin, W.; Bateni, S.M.; Jun, C.; Kim, D.; Liu, S.; Xu, Z.; Ming, W.; Wang, J. A Machine Learning Downscaling Framework Based on a Physically Constrained Sliding Window Technique for Improving Resolution of Global Water Storage Anomaly. *Remote Sens. Environ.* **2024**, *313*, 114359. <https://doi.org/10.1016/j.rse.2024.114359>.
38. Zhang, G.; Xu, T. *Global high-resolution water storage anomaly dataset (2002–2022)*; National Tibetan Plateau/Third Pole Environment Data Center: Beijing, China, 2024. <https://doi.org/10.11888/Terre.tpd.300962>.
39. Ma, H.; Liang, S. Development of the GLASS 250-m Leaf Area Index Product (Version 6) from MODIS Data Using the Bidirectional LSTM Deep Learning Model. *Remote Sens. Environ.* **2022**, *273*, 112985. <https://doi.org/10.1016/j.rse.2022.112985>.
40. Yamazaki, D.; Ikeshima, D.; Tawatari, R.; Yamaguchi, T.; O’Loughlin, F.; Neal, J.C.; Sampson, C.C.; Kanae, S.; Bates, P.D. A High-Accuracy Map of Global Terrain Elevations. *Geophys. Res. Lett.* **2017**, *44*, 5844–5853. <https://doi.org/10.1002/2017GL072874>.
41. Yamazaki, D.; Ikeshima, D.; Sosa, J.; Bates, P.D.; Allen, G.H.; Pavelsky, T.M. MERIT Hydro: A High-Resolution Global Hydrography Map Based on Latest Topography Dataset. *Water Resour. Res.* **2019**, *55*, 5053–5073. <https://doi.org/10.1029/2019WR024873>.
42. Zhang, Q.; Miao, C.; Su, J.; Gou, J.; Hu, J.; Zhao, X.; Xu, Y. A New High-Resolution Multi-Drought-Index Dataset for Mainland China. *Earth Syst. Sci. Data* **2025**, *17*, 837–853. <https://doi.org/10.5194/essd-17-837-2025>.
43. Yang, J.; Huang, X. The 30m Annual Land Cover Dataset and Its Dynamics in China from 1990 to 2019. *Earth Syst. Sci. Data* **2021**, *13*, 3907–3925. <https://doi.org/10.5194/essd-13-3907-2021>.
44. Wang, Z.; Chen, W.; Piao, J.; Cai, Q.; Chen, S.; Xue, X.; Ma, T. Synergistic Effects of High Atmospheric and Soil Dryness on Record-Breaking Decreases in Vegetation Productivity over Southwest China in 2023. *npj Clim. Atmos. Sci.* **2025**, *8*, 6–16. <https://doi.org/10.1038/s41612-025-00895-3>.
45. Chang, X.; Feng, Q.; Ning, T.; Li, Z.; Yang, L.; Zhou, H. Controls and Intermediate Processes of Regional Water Use Efficiency in Northwest China. *J. Hydrol.* **2025**, *663*, 134118. <https://doi.org/10.1016/j.jhydrol.2025.134118>.
46. Liu, Q.; Gui, D.; Zhang, L.; Niu, J.; Dai, H.; Wei, G.; Hu, B.X. Simulation of Regional Groundwater Levels in Arid Regions Using Interpretable Machine Learning Models. *Sci. Total Environ.* **2022**, *831*, 154902. <https://doi.org/10.1016/j.scitotenv.2022.154902>.
47. Ding, K.; Zhao, X.; Cheng, J.; Yu, Y.; Luo, Y.; Couchot, J.; Zheng, K.; Lin, Y.; Wang, Y. GRACE/ML-Based Analysis of the Spatiotemporal Variations of Groundwater Storage in Africa. *J. Hydrol.* **2025**, *647*, 132336. <https://doi.org/10.1016/j.jhydrol.2024.132336>.
48. Xiong, H.; Wang, J.; Yang, C.; Li, S.; Li, X.; Xiong, R.; Wang, Y.; Ma, C. Critical Role of Vegetation and Human Activity Indicators in the Prediction of Shallow Groundwater Quality Distribution in Jiangnan Plain with LightGBM Algorithm and SHAP Analysis. *Chemosphere* **2025**, *376*, 144278. <https://doi.org/10.1016/j.chemosphere.2025.144278>.
49. Razavi-Termeh, S.V.; Sadeghi-Niaraki, A.; Ali, F.; Pirasteh, S.; Shirmohammadi, M.; Choi, S.-M. Spatially Explicit and Interpretable GeoAI Models for Understanding Factors Controlling Groundwater Availability. *J. Hydrol.* **2026**, *665*, 134683. <https://doi.org/10.1016/j.jhydrol.2025.134683>.
50. Zhang, Q.; Gao, X.; Khan, S.U.; Zhou, Z.; He, Z.; Liu, F. Urban Polycentricity, Spatial Compactness, and Carbon Emission Efficiency in China: An Ensemble Machine Learning Evaluation. *Sustain. Cities Soc.* **2026**, *142*, 107306. <https://doi.org/10.1016/j.scs.2026.107306>.
51. Breiman, L. Random Forests. *Mach. Learn.* **2001**, *45*, 5–32. <https://doi.org/10.1023/A:1010933404324>.
52. Chen, T.; Guestrin, C. XGBoost: A Scalable Tree Boosting System. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*; ACM: San Francisco, CA, USA, 8 March 2016; pp. 785–794.

53. Ke, G.; Meng, Q.; Finley, T.; Wang, T.; Chen, W.; Ma, W.; Ye, Q.; Liu, T.-Y. LightGBM: A Highly Efficient Gradient Boosting Decision Tree. In Proceedings of the 31st International Conference on Neural Information Processing Systems, Long Beach, CA, USA, 4–9 December 2017; pp. 3149–3157.
54. Prokhorenkova, L.; Gusev, G.; Vorobev, A.; Dorogush, A.V.; Gulin, A. CatBoost: Unbiased Boosting with Categorical Features. In Proceedings of the 32nd International Conference on Neural Information Processing Systems, Montréal, QC, Canada, 3–8 December 2018; pp. 6638–6648.
55. Friedman, J.H. Greedy Function Approximation: A Gradient Boosting Machine. *Ann. Stat.* **2001**, *29*, 1189–1232. <https://doi.org/10.1214/aos/1013203451>.
56. Wolpert, D.H. Stacked Generalization. *Neural Netw.* **1992**, *5*, 241–259. [https://doi.org/10.1016/S0893-6080\(05\)80023-1](https://doi.org/10.1016/S0893-6080(05)80023-1).
57. Kanani-Sadat, Y.; Safari, A.; Nasser, M.; Homayouni, S. A Novel Explainable Stacking Ensemble Model for Estimating Design Floods: A Data-Driven Approach for Ungauged Regions. *Adv. Eng. Inf.* **2025**, *66*, 103429. <https://doi.org/10.1016/j.aei.2025.103429>.
58. Akiba, T.; Sano, S.; Yanase, T.; Ohta, T.; Koyama, M. Optuna: A Next-Generation Hyperparameter Optimization Framework. In Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Anchorage, AK, USA, 4–8 August 2019; pp. 2623–2631. <https://doi.org/10.1145/3292500.3330701>.
59. Hoerl, A.E.; Kennard, R.W. Ridge Regression: Biased Estimation for Nonorthogonal Problems. *Technometrics* **2000**, *42*, 81–86. <https://doi.org/10.2307/1271436>.
60. Lundberg, S.M.; Lee, S.-I. A Unified Approach to Interpreting Model Predictions. In Proceedings of the 31st International Conference on Neural Information Processing Systems, Long Beach, CA, USA, 4–9 December 2017; pp. 4765–4774.
61. Lundberg, S.M. From Local Explanations to Global Understanding with Explainable AI for Trees. *Nat. Mach. Intell.* **2020**, *2*, 56–67. <https://doi.org/10.1038/s42256-019-0138-9>.
62. Yang, J.; Li, R.; Lei, Y.; Ning, K.; Li, S.; Zhang, Y.; Hou, J.; Lang, T.; Cao, Y.; Li, W.; et al. Global Soil Water Stable Isotope Dataset. *Sci. Data* **2026**, *13*, 415. <https://doi.org/10.1038/s41597-026-07262-8>.
63. Liang, H.; Jiapaer, G.; Chang, C.; Yu, T.; Zhang, L.; Feng, P.; Lin, K.; Ju, T.; Jiang, X.; De Maeyer, P.; et al. Vegetation in Central Asia Is More Sensitive to Soil Moisture Stress than to Precipitation and Vapor Pressure Deficit Stresses. *Agric. For. Meteorol.* **2026**, *383*, 111140. <https://doi.org/10.1016/j.agrformet.2026.111140>.
64. Li, Y.; Huang, S.; Chen, D.; Li, J.; Leng, G.; Huang, Q.; Wang, Z.; Peng, J. Quantifying the Dampening Effect of Soil Moisture on Drought Propagation in Northern Ecosystems. *J. Hydrol.* **2026**, *674*, 135518. <https://doi.org/10.1016/j.jhydrol.2026.135518>.
65. Xia, H.; Zhang, F.; Ciais, P.; Stoy, P.C.; Peñuelas, J.; Lian, X.; Wang, Y.-P.; Makowski, D.; Luo, Y.; Niu, S.; et al. Higher Optimal Temperature for Vegetation Transpiration than for Photosynthesis. *Nat. Plants* **2026**, *12*, 703–718. <https://doi.org/10.1038/s41477-026-02263-2>.
66. Zhao, M.; Aa, G.; Liu, Y.; Konings, A. Evapotranspiration Frequently Increases during Droughts. *Nat. Clim. Change* **2022**, *12*, 1024–1030. <https://doi.org/10.1038/s41558-022-01505-3>.
67. Yang, D.; Wu, L.; Zhang, Y.; Wei, H.; Chen, D.; Xiong, L.; Du, J.; Jia, J. Subsurface-Fed Transpiration Drives Surface Energy Partitioning in Soil-Limited Karst Systems. *J. Hydrol.* **2025**, *663*, 134159. <https://doi.org/10.1016/j.jhydrol.2025.134159>.
68. Hsu, H.; Dirmeyer, P.A. Soil Moisture-Evaporation Coupling Shifts into New Gears under Increasing CO₂. *Nat. Commun.* **2023**, *14*, 1162. <https://doi.org/10.1038/s41467-023-36794-5>.
69. Wang, L.; Good, S.P.; Caylor, K.K. Global Synthesis of Vegetation Control on Evapotranspiration Partitioning. *Geophys. Res. Lett.* **2014**, *41*, 6753–6757. <https://doi.org/10.1002/2014GL061439>.
70. Scott, R.L.; Biederman, J.A. Partitioning Evapotranspiration Using Long-Term Carbon Dioxide and Water Vapor Fluxes. *Geophys. Res. Lett.* **2017**, *44*, 6833–6840. <https://doi.org/10.1002/2017GL074324>.
71. Liu, Z.; Wang, Y.; Yu, P.; Xu, L.; Yu, S. Environmental and Canopy Conditions Regulate the Forest Floor Evapotranspiration of Larch Plantations. *For. Ecosyst.* **2022**, *9*, 100058. <https://doi.org/10.1016/j.fecs.2022.100058>.
72. Liu, Y.; Lian, J.; Behzad, H.M.; Nie, Y.; Pan, Z.; Chen, H. Environmental Drivers of Drought Effects on Vegetation Growth across Southwest China: Insights from an Integrated Soil Moisture Threshold and Effect Size Framework. *J. Environ. Manag.* **2026**, *404*, 129443. <https://doi.org/10.1016/j.jenvman.2026.129443>.
73. Fu, Z.; Ciais, P.; Wigneron, J.-P.; Gentile, P.; Feldman, A.F.; Makowski, D.; Viovy, N.; Kemanian, A.R.; Goll, D.S.; Stoy, P.C.; et al. Global Critical Soil Moisture Thresholds of Plant Water Stress. *Nat. Commun.* **2024**, *15*, 4826. <https://doi.org/10.1038/s41467-024-49244-7>.
74. Zheng, X.; Li, Y.; Zhou, Q.; Zhao, Y.; Cai, L.; Shi, C.; Chen, Y. Rock Fissure Water Dominates the Water Utilization Strategies of Woody Plants in Karst Epikarst. *J. Hydrol.* **2026**, *674*, 135570. <https://doi.org/10.1016/j.jhydrol.2026.135570>.

75. Qiu, Y.; Zhang, F.; Gao, L.; He, Z.; Xiong, H.; Peng, L.; Wang, Z.; Cui, H.; Su, C.; Zhang, D.; et al. Uncovering the Dynamic Role of Bedrock-Stored Water in Ecosystem Evapotranspiration. *J. Hydrol.* **2026**, *668*, 134987. <https://doi.org/10.1016/j.jhydrol.2026.134987>.
76. Ehlert, R.S.; Hahm, W.J.; Dralle, D.N.; Rempe, D.M.; Allen, D.M. Bedrock Controls on Water and Energy Partitioning. *Water Resour. Res.* **2024**, *60*, e2023WR036719. <https://doi.org/10.1029/2023WR036719>.
77. Chen, G.; Zhang, K.; Li, Y.; Feng, J.; Bogaard, T. Empowering a Coupled Hydrological-Geotechnical Model to Simulate Long-Term Vegetation Dynamics and Their Impact on Catchment-Scale Flood and Landslide Hazards. *J. Hydrol.* **2025**, *658*, 133225. <https://doi.org/10.1016/j.jhydrol.2025.133225>.
78. Zhan, Y.; Guo, Z.; Podgorski, J.; Zeng, Z.; Xu, P.; Peng, L.; Chen, K.; Wu, R.; Ding, C.; Andrews, C.; et al. Changes in Meat Consumption Can Improve Groundwater Quality. *Nat. Food* **2025**, *6*, 703–714. <https://doi.org/10.1038/s43016-025-01188-x>.
79. Chen, H.; Han, Z.; Yan, X.; Bai, Z.; Li, Q.; Wu, P. Impacts of Land Use on Phosphorus and Identification of Phosphate Sources in Groundwater and Surface Water of Karst Watersheds. *J. Environ. Manag.* **2024**, *366*, 121919. <https://doi.org/10.1016/j.jenvman.2024.121919>.
80. Dong, P.; Zuo, R.; Tang, M.; He, C.; Li, J.; Liao, T.; Gong, Y.; Zhang, S.; Gong, J.; Yi, Y. Scenario Simulation of Tea Expansion Impacts in Karst Ecosystems. *Ecosyst. Health Sustain.* **2026**, *12*, 0521. <https://doi.org/10.34133/ehs.0521>.
81. Colliander, A.; Jackson, T.J.; Chan, S.K.; O'Neill, P.; Bindlish, R.; Cosh, M.H.; Caldwell, T.; Walker, J.P.; Berg, A.; McNairn, H.; et al. An Assessment of the Differences between Spatial Resolution and Grid Size for the SMAP Enhanced Soil Moisture Product over Homogeneous Sites. *Remote Sens. Environ.* **2018**, *207*, 65–70. <https://doi.org/10.1016/j.rse.2018.02.006>.
82. Zhang, Q.; Zhang, K.; Bárdossy, A.; Li, Y.; Wu, N. Improving Representation of Hydrological Process Heterogeneity in Grid-Xin'anjiang Model through a Stepwise Approach. *J. Hydrol.* **2025**, *655*, 132897. <https://doi.org/10.1016/j.jhydrol.2025.132897>.
83. Zhang, Q.; Zhang, K.; Chao, L.; Chen, X.; Wu, N. A Unified Runoff Generation Scheme for Applicability across Different Hydrometeorological Zones. *Environ. Modell. Softw.* **2024**, *180*, 106138. <https://doi.org/10.1016/j.envsoft.2024.106138>.

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.