

Article

Revealing Driving Factors of Water Use Efficiency in the Huang–Huai–Hai Plain Using an Optimized XGBoost-SHAP Model

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Abstract

A comprehensive understanding of the spatiotemporal evolution of water use efficiency (WUE) and its driving mechanisms is essential for sustainable water resource management in the Huang–Huai–Hai Plain (HHHP), a critical agricultural production base in northern China. Based on multi-source remote sensing datasets from 2001 to 2024, this study adopted the Sen-MK trend test and optimized XGBoost-SHAP framework to characterize the spatiotemporal variations in WUE and quantify corresponding driving forces: (1) WUE exhibited a predominantly rising trend across 78.53% of the study area, with significant increases concentrated in the southwestern Shandong hilly region; high WUE values ($1.68\text{--}1.74\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$) occurred in the eastern Shandong hills and southwestern North China Plain, while low values ($1.50\text{--}1.56\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$) were found in the northern North China Plain and southeastern Bohai Bay area. (2) Among vegetation types, shrubland showed the highest multi-year mean WUE ($1.75\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$) and wetland the lowest ($1.34\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$); cropland displayed the most rapid increasing trend ($0.0045\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}\cdot\text{a}^{-1}$), while wetland showed a decreasing trend. (3) The HHHP showed low interannual volatility and strong persistence of WUE, with stable interannual WUE and historical persistence suggesting that the increasing trend may continue in most areas. (4) Spatial variation in WUE is primarily driven by NDVI and temperature, with NDVI having the greatest influence, accounting for approximately 40.36% of the vegetated area, while temperature accounts for 26.43%, ranking second; precipitation and the aridity index exerted secondary regulatory effects, with positive effects mainly in the Huang–Huai Plain and negative effects in the North China Plain. This study elucidates the evolutionary mechanisms of WUE under coupled climate–vegetation influences, providing critical scientific evidence for optimizing regional water resource allocation and management and promoting sustainable agricultural practices in this water-limited region.



Academic Editor: Songhao Shang

Received: 15 May 2026

Revised: 3 July 2026

Accepted: 6 July 2026

Published: 10 July 2026

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Keywords: Huang–Huai–Hai Plain; XGBoost-SHAP model; water use efficiency; driving mechanisms; NDVI

1. Introduction

In terrestrial ecosystems, WUE is defined as the ratio of gross primary productivity (GPP) to evapotranspiration (ET). This index quantifies the degree of coupling between

the carbon and water cycles, revealing vegetation's capacity to fix carbon per unit of water that it consumes [1,2]. In the context of intensified global climate change and intensive human disturbance, clarifying the spatiotemporal dynamics of WUE is crucial for evaluating ecosystem resilience, identifying ecosystem feedbacks to environmental changes, and supporting sustainable regional water resource management [3,4]. As one of China's most important grain-producing regions and densely populated areas, the ecosystem stability of the HHHP is closely associated with national food security and water resource security [5]. However, the region is confronted with multiple ecological stressors, including water scarcity, climate warming and drying, and intensive land use activities, making ecosystem WUE a core metric to characterize regional eco-hydrological dynamics and ecosystem adaptive capacity [6]. As a comprehensive composite indicator, WUE integrates two functionally distinct ecological processes, which impede accurate identification of physiological mechanisms governing carbon–water coupling. To overcome this limitation, WUE is decomposed into two components: photosynthetic–transpiration coupling efficiency (GPP/T) and the transpiration allocation ratio (T/ET) [7]. GPP/T quantifies the amount of carbon fixed per unit of water lost through transpiration, reflecting the intrinsic photosynthetic water use efficiency of vegetation; T/ET represents the proportion of transpiration relative to total ecosystem evapotranspiration, which is primarily determined by vegetation structure and surface energy balance rather than photosynthetic activity itself [8]. The decomposition of WUE into GPP/T and T/ET enables the differentiation of driving sources for WUE variations, namely improved photosynthetic water use efficiency or altered water partitioning between transpiration and evaporation [9]. For example, CO_2 fertilization may enhance GPP/T , whereas vegetation cover may increase T/ET by suppressing soil evaporation; however, the two scenarios require divergent water management approaches with separate ecological implications. Therefore, systematically revealing the spatiotemporal patterns of WUE across the HHHP and the spatial heterogeneity of its dominant driving factors is not only a scientific necessity for deepening our understanding of ecological hydrological processes in typical agricultural regions but also an urgent practical requirement to provide a scientific basis for regional climate change adaptation and optimization of water and soil resource management policies [10].

In recent years, advancements in remote sensing and modeling technologies have significantly facilitated spatiotemporal dynamic studies of WUE from regional to global scales. Extensive research indicates that the spatiotemporal patterns of WUE show substantial spatial heterogeneity instead of consistent trends. Globally, WUE generally shows an increasing trend, primarily attributed to the fertilization effect caused by elevated atmospheric CO_2 concentrations and vegetation greening [11,12]. In arid and semiarid regions, for instance, water availability generally serves as the primary constraint on WUE variability, whose dynamics are highly sensitive to Pre fluctuations [9], whereas in ecologically fragile areas or watersheds subject to intense human activities, WUE may exhibit complex nonlinear changes or even declining trends [13,14]. Studies on major ecological zones in China have also revealed similar spatial heterogeneity. For example, vegetation restoration on the Loess Plateau significantly improved WUE, while the Mongolian Plateau experienced a decreasing trend in ecosystem carbon utilization efficiency, driven by the combined impacts of climate change and human activities [12,15]. These studies underscore the necessity of conducting refined WUE dynamic assessments within specific geographic units.

The WUE of ecosystems is significantly influenced by vegetation types, as different vegetation types have fundamentally distinct physiological structures, photosynthetic pathways, and water-use strategies. Global integrated analyses indicate substantial variations in WUE among major ecosystems such as forests, grasslands, and farmlands, with typically higher WUE in farmlands and lower in forests. These differences are primarily determined

by ecosystem type and climatic conditions [16,17]. For example, on the Qinghai–Tibet Plateau, warming experiments revealed distinctly different impacts on carbon and WUE in alpine meadows versus artificial grasslands [18]; in karst regions, the WUE of different vegetation types also exhibited significant variations in response to climatic factors [19]. Furthermore, vegetation succession or management measures can also alter WUE. In subtropical forests, for example, an increase in tree species diversity can lead to higher soil microbial carbon use efficiency, which may indirectly affect ecosystem-level carbon–water coupling [20]. These studies highlight the necessity to account for vegetation type heterogeneity and its unique response mechanisms when analyzing regional WUE.

Studies have demonstrated that WUE is co-regulated by climatic factors (e.g., T_{em} , P_{re} , and vapor pressure deficit), biological factors (such as leaf area index (LAI) and NDVI), and anthropogenic factors (including land use change, nitrogen deposition, and agricultural management practices), with the relative significance of these factors varying spatially and temporally [21,22]. For instance, a rise in T_{em} may reduce WUE by increasing transpiration (T) and water loss, whereas an increase in vegetation coverage (e.g., NDVI) typically enhances WUE through elevated photosynthesis [23]. The role of human factors is becoming increasingly prominent. Nitrogen deposition has been proven to augment the positive impact of CO_2 fertilization on WUE in China [24], while different agricultural management practices (e.g., fertilization) can significantly modify the carbon utilization efficiency of soil microorganisms, thereby affecting WUE [25]. In recent years, explainable machine learning methods, such as the SHAP algorithm and structural equation modeling (SEM), have been increasingly used to quantify the contributions and interactions of multiple factors, thereby revealing the complexity of driving mechanisms. For example, in the Loess Plateau region, the interplay between climate and topography accounts for a greater proportion of the spatial variation in WUE than any single factor [12,26].

Although existing studies have extensively explored the spatiotemporal dynamics and driving mechanisms of WUE at multiple scales, systematic and targeted research focusing on the HHHP remains inadequate. First, although national-scale analyses have revealed an overall increasing trend in WUE, such macroscopic perspectives often obscure the internal heterogeneity within key agroecological zones. Specifically, existing studies lack a detailed characterization of the long-term spatial and temporal changes in WUE across the HHHP—a typical high-intensity human–land coupling region—and particularly fail to systematically decouple WUE into critical intermediate physiological processes, such as “photosynthetic–transpiration coupling efficiency (GPP/T)” and “transpiration allocation partitioning ratio (T/ET)”, thereby limiting a mechanistic understanding of the complete carbon–water coupling chain [27,28]. Secondly, although the inherent differences in WUE across vegetation types have been widely documented [29], under the complex landscape pattern of the HHHP—dominated by farmland interspersed with patches of natural vegetation—quantitative comparisons of long-term WUE temporal trends between natural vegetation (e.g., forests, shrubs, grasslands) and cultivated vegetation (primarily crops) remain insufficiently explored. Finally, although interpretable machine learning methods (e.g., SHAP algorithms) have emerged as powerful tools for quantifying WUE drivers [30,31], the HHHP has yet to fully integrate hyperparameter optimization frameworks with spatially explicit analyses to accurately quantify the nonlinear contributions and spatial heterogeneity effects of multiple factors, such as climate and vegetation, on WUE. Accordingly, this study aims to (1) investigate the spatiotemporal evolution patterns of WUE and its key components (GPP , ET) as well as intermediate processes (GPP/T , T/ET) in the HHHP ecosystem from 2001 to 2024; (2) quantitatively compare temporal WUE trends among different vegetation types in the study area; (3) and adopt an interpretable machine learning approach with integrated optimized parameters to identify the spatial

heterogeneity of dominant driving factors influencing spatiotemporal changes in WUE within the HHHP ecosystem.

2. Overview of the Study Area

The HHHP is situated in eastern China, covering provinces such as Henan, Shandong, Anhui, Jiangsu, and Hebei, with a total land area of approximately 300,000 square kilometers. As a large alluvial plain formed by the Yellow, Huaihai and Haihe Rivers, it serves as a pivotal agricultural and ecological region in northern China (Figure 1). The area features diverse topography, divided into Bohai Gulf Zone, North China Plain Zone, Shandong Hill Zone, and Huang–Huai Plain Zone (Figure 1a). The zoning is based on the agricultural resource and environment classification of China, which adopts a county-level mapping unit and a two-level hierarchical approach using the dominant factor method, following a comprehensive analysis of regional agricultural production characteristics, suitability, and environmental conditions. The first-level zones are delineated according to climatic conditions and geotectonic differentiation, while the second-level zones are further subdivided based on disparities in water resources, land resources, and environmental conditions [32]. The land use in the region is dominated by agricultural ecosystems, with farmland occupying approximately 85.55% of the total study area. Forests are mainly concentrated in hilly regions, where grasslands and wetlands are mainly concentrated in coastal zones (Figure 1b). The HHHP experiences a temperate monsoon climate, with significant spatial heterogeneity in water and heat conditions. The aridity index exhibits an increasing trend from south to north (Figure 1c). High-value areas of the NDVI are located in the southern plains and eastern hills (Figure 1d). Potential ET is lowest along the coast (Figure 1e). Pre decreases from the southeast to the northwest (Figure 1f), and relative humidity (Rhu) follows a distribution pattern similar to that of Pre (Figure 1g). Temps is generally warmer in the south compared to the north (Figure 1h).

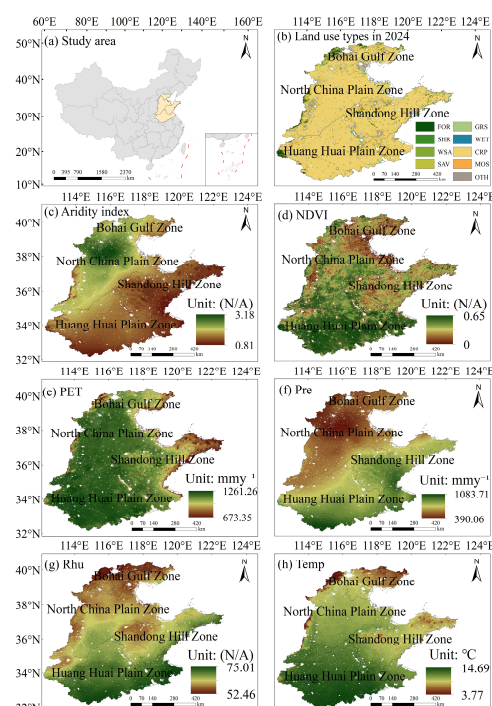


Figure 1. Spatial distribution of the study area and key environmental variables in the North China Plain. (a) Study area location within China (highlighted in yellow); (b) land use types in 2024; (c–h) multiyear mean values of aridity index, NDVI, PET, Pre, Rhu, and Temp, respectively; N/A denotes that the data unit is dimensionless.

3. Data and Methods

3.1. Data Sources and Processing

The data adopted three core ecological variables, namely GPP, ET, and T, which were retrieved from Moderate Resolution Imaging Spectroradiometer (MODIS) satellite datasets (NASA, Washington, DC, USA). Specifically, GPP and ET were derived from the MOD17A2H (Version 6.1) and MOD16A2GF (Version 6.1) products, respectively. It should be noted that T (transpiration) cannot be directly obtained from remote-sensing products; it was estimated via ET partitioning using the Two-Source Energy Balance model coupled to the Soil Moisture (TSEB-SM) model [33]. We acquired all MODIS datasets from the NASA Level-1 and Atmosphere Archive & Distribution System (LAADS DAAC) platform (Greenbelt, MD, USA). Land use/land cover data were derived from the MCD12Q1 (Version 6.1) product, also provided by the NASA LAADS DAAC. The NDVI, aridity index (AI), and potential evapotranspiration (PET) were obtained from the National Tibetan Plateau Science Data Center (TPDC) (Beijing, China). The NDVI dataset is based on the SPOT/VEGETATION and MODIS NDVI products. The AI and PET datasets are derived from the Global Aridity Index and Potential Evapotranspiration (Global-AI_PET_v3) database (the AI dataset is based on China's 1-km monthly PET and precipitation PRE data and is calculated using the ratio method, where the AI value is the ratio of annual potential evapotranspiration to annual precipitation). Meteorological variables, including mean annual temperature (Tem), precipitation (Pre), and relative humidity (Rhu), were collected from the National Glacier, Permafrost and Desert Science Data Center (NCDC) (Lanzhou, China). Detailed information about all data sources is provided in Table 1. The study period spans from 2001 to 2024.

Table 1. Summary of data used in this study (Note: “—” indicates that the unit or temporal resolution is not applicable).

Dataset	Version	Temporal Coverage	Unit	Spatial Resolutions	Temporal Resolutions	Data Source
GPP	6.1	2001–present	$\text{gCm}^{-2}\text{y}^{-1}$	500 m	8 days	https://ladsweb.modaps.eosdis.nasa.gov/ , accessed on 1 April 2026
T	6.1	2001–present	mmy^{-1}	500 m	8 days	
ET	6.1	2001–present	mmy^{-1}	500 m	8 days	
Land use	6.1	2001–present	—	500 m	annual scale	https://doi.org/10.5067/MODIS/MCD12Q1.006 , accessed on 18 April 2026
NDVI	—	2001–2025	—	1 km	annual scale	https://search.earthdata.nasa.gov/ , accessed on 3 May 2026
AI	3	1901–2024	—	1 km	annual scale	https://www.tpdc.ac.cn/home , accessed on 5 May 2026
PET	3	1901–2024	mm	1 km	monthly scale	
Tem	—	1980–2024	°C	1 km	monthly scale	https://www.ncdc.ac.cn/portal/ , accessed on 7 May 2026
Pre	—	1980–2024	mm	1 km	monthly scale	
Rhu	—	1980–2024	—	1 km	annual scale	

This study implemented systematic preprocessing of multi-source data. First, multi-source raw datasets (HDF, NetCDF, raster formats) were standardized via format conversion and batch merging. Subsequently, using the spatial analysis functions of ArcPy, all data layers were uniformly clipped to the geographic extent of the HHHP research

region. To ensure spatial consistency, the original 1-km resolution data were resampled and standardized to a 500-m resolution. Finally, key ecological indicators such as WUE were calculated based on pixel-level analysis, followed by time series synthesis and outlier removal, resulting in the construction of a standardized dataset for driving mechanism analysis. The calculation steps for the annual mean values of GPP, ET, and T are as follows: First, each annual dataset comprises 46 product periods; the values of the first 45 eight-day composites were multiplied by 8 and summed. Second, it is determined whether the year is a leap year. If it is a leap year, the 46th period is multiplied by 6; if it is not a leap year, it is multiplied by 5. Finally, the above results are accumulated and multiplied by the corresponding coefficient to obtain the annual mean value of each variable. After that, outliers in the annual mean data are removed, specifically values less than 0 or missing values. For precipitation and PET, the annual mean values are obtained by summing the monthly data to yield the annual total. For temperature, the annual mean values are calculated by arithmetically averaging the monthly data.

The pixel-wise extraction workflow of WUE, GPP, ET and intermediate indicators for different vegetation types is described below. Firstly, the pixel-by-pixel positions of different vegetation types in the Huang–Huai–Hai region from 2001 to 2024 are extracted. Then, based on the pixel-by-pixel position data of different vegetation types in each year, WUE, GPP, ET, and their intermediate process data are extracted for each year.

3.2. Methods

3.2.1. WUE

WUE can be decomposed into the product of T-based WUE and the T ratio [7]. The formula is provided below:

$$WUE = \frac{GPP}{ET} = \left(\frac{GPP}{T}\right) \times \left(\frac{T}{ET}\right) = WUE_T \times \left(\frac{T}{ET}\right) \quad (1)$$

3.2.2. Sen + MK Method

Analyses were conducted using the Theil–Sen Median and Mann–Kendall tests to explore the spatiotemporal trends of WUE in the HHHP from 2001 to 2024. These methods are reliable for capturing monotonous temporal trends and are robust against outliers. The mathematical formula for the Theil–Sen Median is shown below:

$$Sen = Median\left(\frac{X_j - X_i}{j - i}\right), 2001 \leq i < j \leq 2024 \quad (2)$$

where X denotes WUE. If $Sen > 0$, WUE exhibits an increasing tendency; conversely, it denotes a downward trend. The Mann–Kendall formula is listed as follows:

Let $\{X_i\}, i = 2001, 2002, \dots, 2024$, and the Z-statistic is defined as:

$$Z = \begin{cases} \frac{S-1}{\sqrt{s(S)}}, S > 0 \\ 0, S = 0 \\ \frac{S+1}{\sqrt{s(S)}}, S < 0 \end{cases} \quad \text{where, } S = \sum_{j=1}^{n-1} \sum_{i=j+1}^n \text{sgn}(X_j - X_i) \quad (3)$$

There is no “conclusion” in the data of this study, so the variance calculation formula is as follows:

$$\text{sgn}(X_j - X_i) = \begin{cases} 1, X_j - X_i > 0 \\ 0, X_j - X_i = 0 \\ -1, X_j - X_i < 0 \end{cases}, \text{Var}(S) = \frac{n(n-1)(2n+5)}{18} \quad (4)$$

The results of the Mann–Kendall test at the 0.05 confidence level are classified as significant fluctuations ($Z \geq 1.96$ or $Z \leq -1.96$) and insignificant variations ($-1.96 < Z < 1.96$).

3.2.3. Hurst Exponent Analysis

To evaluate the historical persistence characteristics of interannual WUE dynamics, the Hurst exponent (H) of WUE from 2001 to 2024 was calculated using rescaled range analysis (R/S analysis) [34]. The index ranges between 0 and 1 and quantifies the long-term trend persistence of time-series variables. An H value between 0 and 0.5 indicates anti-persistence, suggesting a potential reversal in historical trends. An H value of exactly 0.5 indicates a random walk process without discernible patterns. Conversely, an H value between 0.5 and 1 indicates positive long-term persistence, suggesting that historical trends may continue. Notably, the 24-year time series restricts the robustness of R/S analysis; thus, results only reflect historical trend persistence instead of deterministic future projections. By combining WUE change patterns with the calculated H, the historical persistence of each identified WUE change pattern in the HHHP was classified, as detailed in Table 2.

Table 2. Assessment of WUE variation pattern sustainability in the HHHP.

H Value	Variation Patterns of WUE	WUE Variation Pattern Sustainability
>0.5	Significant increase	Sustained and significant increase
>0.5	Slight increase	Sustained and slight increase
>0.5	Slight decrease	Sustained and slight decrease
>0.5	Significant decrease	Sustained and significant decrease
<0.5	Failed to pass a significant change	No clear persistence direction

3.2.4. Analysis of Interannual Fluctuation Intensity

The coefficient of variation (CV), calculated as the ratio of the standard deviation to the mean, was used to quantify the relative amplitude of interannual fluctuations in WUE and evaluate its temporal stability [35]. Based on the CV value, the fluctuation intensity of each pixel was classified into five levels: high volatility ($CV \geq 0.2$), medium–high volatility ($0.16 \leq CV < 0.2$), medium volatility ($0.12 \leq CV < 0.16$), medium–low volatility ($0.08 \leq CV < 0.12$), and low volatility ($CV \leq 0.08$). The above classification methods were based on the natural discontinuity method.

3.2.5. Optimization Parameters for XGBoost Model

XGBoost Model

This study utilized the XGBoost (Extreme Gradient Boosting) model, an integrated learning algorithm constructed on the gradient boosting system. By sequentially constructing multiple weak learners, it progressively reduces model bias and residuals, effectively mitigating underfitting issues [36]. The algorithm is widely adopted for its outstanding predictive performance, high computational efficiency, and excellent scalability across various machine learning tasks, including regression and classification [24]. Methodologically, while the XGBoost algorithm itself is well-established, the innovation of our approach lies in the targeted integration of this powerful algorithm with SHAP analysis to address a specific and complex ecological question—quantifying the nonlinear and spatially heterogeneous driving mechanisms of WUE across the HHHP. This combination allows us to move beyond the limitations of traditional linear regression or correlation analyses, which often fail to capture the high-order interactions and ecological thresholds that characterize eco-hydrological processes.

To justify the selection of XGBoost as the core predictive model, we considered its well-documented advantages over alternative machine learning algorithms in ecological and hydrological modeling. Compared with traditional regression approaches such as Multiple Linear Regression (MLR), XGBoost inherently accommodates complex nonlinear relationships, multicollinearity, and high-order interactions among driving factors—common characteristics of eco-hydrological datasets. Relative to other ensemble methods like Random Forest (RF), XGBoost employs a gradient-boosting framework that sequentially corrects residual errors, often yielding competitive or superior predictive accuracy in complex ecological datasets. Furthermore, when contrasted with LightGBM and CatBoost, XGBoost offers a more mature ecosystem of interpretability tools, particularly its seamless integration with SHAP for model explanation—a critical requirement for our study's objective of elucidating driver mechanisms. The algorithm's built-in regularization also provides effective protection against overfitting when modeling spatially heterogeneous environmental data. On the basis of these theoretical and practical considerations, XGBoost was selected as the final predictive model for subsequent SHAP-based interpretation.

To improve prediction accuracy and generalization performance, we combined 10-fold cross-validation with random search to implement hyperparameter tuning [30]. Specifically, the model underwent multiple rounds of iterative training and evaluation, ultimately selecting the optimal hyperparameter combination for constructing the final prediction model.

Seven primary datasets were used to develop the model, with WUE as the dependent variable and NDVI, AI, PET, Temp, Pre, and Rhu as independent variables. The hyperparameter optimization process involved the following steps: First, the data were equally partitioned into 10 subgroups to ensure each subgroup represented the overall data characteristics. Ten training rounds were conducted, with one subgroup serving as the validation set and the remaining nine merged into the training set. After all training cycles were completed, the average performance metrics of model predictions were aggregated. Subsequently, a random search method was employed to sample parameters within a predefined hyperparameter space, using root mean square error (RMSE) and coefficient of determination (R^2) as evaluation metrics to select the optimal hyperparameter set among alternative model configurations. The optimization process was monitored for convergence to ensure that the selected parameters represented a stable optimum rather than a local fluctuation. The optimized XGBoost model achieved an RMSE of 0.043 and an R^2 of 0.85 on the test set, demonstrating its ability to reliably capture the spatiotemporal dynamics of WUE in the HHHP and the heterogeneous impacts of key driving factors. The hyperparameters of the optimized XGBoost model were set as follows: 323 trees, a learning rate of 0.0922, a maximum tree depth of 9, a subsampling ratio of 0.9725, and a feature sampling ratio of 0.993.

SHAP Interpretation Model

SHapley Additive Explanations (SHAP) is a model-agnostic interpretability framework rooted in cooperative game theory. It measures the contribution of each independent input feature to the prediction outcomes of individual machine learning models, addressing the “black box” characteristics of models [12]. While XGBoost delivers state-of-the-art predictive performance, its inherent complexity obscures the internal decision-making logic. This renders the introduction of SHAP critical to the present work, as it functions as an essential “bridge” connecting high-accuracy prediction and model interpretability. By applying SHAP, we can disentangle the complex feature interactions captured by the XGBoost model and explicitly attribute WUE variations to individual drivers. This transforms the modeling framework from a pure predictive tool into an interpretable approach

for identifying dominant driving factors and exploring nonlinear feature–response relationships in eco-hydrology. The method calculates marginal contribution averages (i.e., Shapley values) across various feature combinations to provide consistent and reliable attribution explanations for prediction outcomes. Its computational process adheres to three fundamental axioms: local accuracy (predictions for any sample can be precisely reconstructed from the sum of feature contributions), missingness (zero contribution when features are absent), and consistency (Shapley values should not decrease when model dependence on a feature increases) [37]. In this study, SHAP was used to interpret predictions of WUE by trained XGBoost models. By analyzing the magnitude and sign of Shapley values for driving factors (e.g., Pre, Tem), we quantitatively revealed their directional and intensity impacts on WUE, elucidating nonlinear characteristics and spatial heterogeneity in the relationships between key factors and WUE. The computational formula is as follows:

$$x_i = \sum_{s \in S_i} \frac{(n - |s|)! (|s| - 1)!}{n!} \left[v(s) - v\left(\frac{s}{i}\right) \right] \quad (5)$$

where x_i denotes the payoff of player i , s is a specific coalition in S_i , $|s|$ represents the number of elements within subset s , n refers to the total number of players, $v(s)$ denotes the payoff of coalition s , and $v(s/i)$ stands for the payoff of the coalition obtained by removing player i from s . The formula for calculating the Shapley value is given as follows:

$$y_i = y_{base} + f(x_{i,1}) + f(x_{i,2}) + \dots + f(x_{i,j}) + \dots + f(x_{i,k}) \quad (6)$$

where y_i represents the predicted value of i -th, y_{base} is the mean predicted value across all samples, $x_{i,j}$ is the j -th feature of the i -th sample, $f(x_{i,j})$ denotes the SHAP value of the j -th feature for the i -th sample, and k stands for the total number of input features.

3.2.6. Calculation of Importance Indicators

Notably, while the SHAP value magnitude reflects a feature's marginal contribution, the presence of multicollinearity among driving factors (e.g., Temp and PET) may lead to interaction effects. Our analysis focuses on identifying the dominant driving factor at each pixel, while acknowledging that synergistic effects also play a role in WUE dynamics. Given this premise, on the basis of the SHAP values associated with various driving factors influencing WUE in the HHHP, this study conducted further spatial statistical analysis. The procedure was as follows: First, the magnitude of SHAP values for each driving factor was calculated for individual pixels. Next, by comparing the magnitude of SHAP values of all factors pixel-by-pixel, the maximum SHAP absolute value at each location was identified. Finally, the driving factor corresponding to this maximum value was designated as the dominant driving factor for that pixel. This workflow enabled the spatial identification of dominant drivers governing WUE spatiotemporal variations and revealed their spatial distribution patterns.

4. Results

4.1. Spatiotemporal Dynamic Changes in WUE

4.1.1. Spatial Distribution of WUE

Figure 2 illustrates the spatial distribution of WUE, GPP, ET, and their intermediate processes in the HHHP from 2001 to 2024. High WUE values, ranging from 1.68 to 1.74 g C·m⁻²·mm⁻¹, are predominantly concentrated in the eastern Shandong hilly region and the southwestern part of the North China Plain, while low WUE values, between 1.50 and 1.56 g C·m⁻²·mm⁻¹, are mainly observed in the northern North China Plain and the southeastern Bohai Bay Area. GPP and ET share highly consistent spatial

patterns, both showing a gradual increasing gradient from northwest to southeast, with high-value regions primarily located in the Huang–Huai Plain. The spatial distribution of T shows a pattern comparable to that of WUE, while low T/ET values mainly occur in the Shandong hilly zone, a pattern opposite to the spatial distributions of T and WUE. Low GPP/T ratios are mainly concentrated in the central and eastern lowlands of the North China Plain, while high values are mainly concentrated along the western edge of the region and the southeastern Shandong hilly region.

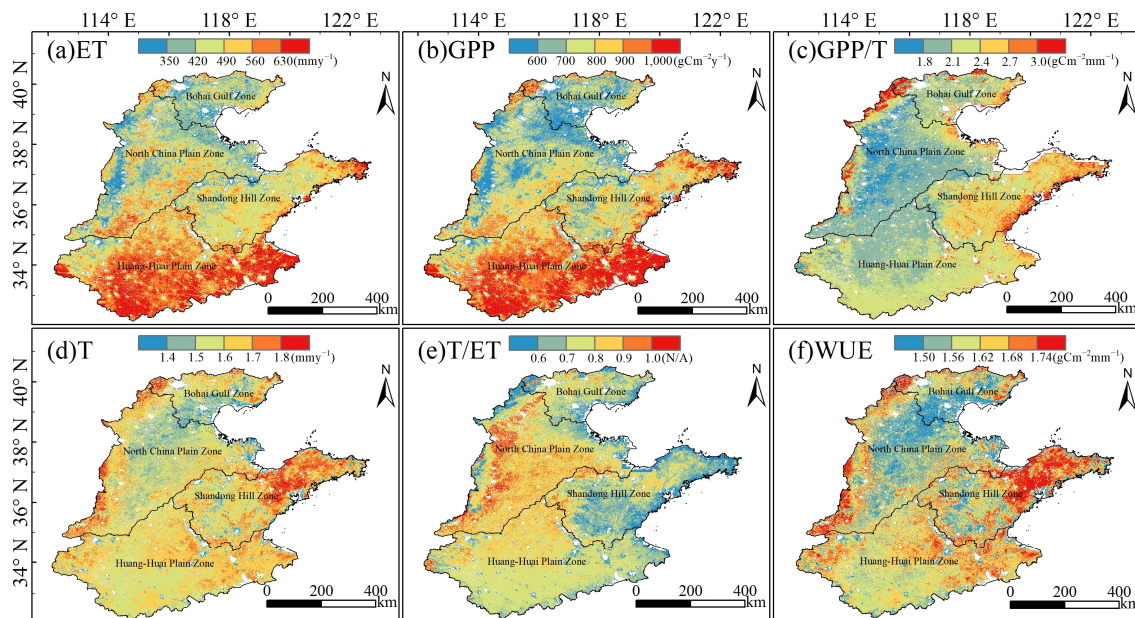


Figure 2. Spatial distribution of WUE, GPP, ET, and their intermediate processes. Panels (a–f) represent the multi-year average (2001–2024) of (a) ET, (b) GPP, (c) GPP/T, (d) T, (e) T/ET, and (f) WUE, respectively.

4.1.2. Spatial Variation Trends of WUE

Figure 3 depicts the temporal variation trends of WUE, GPP, ET, and their intermediate processes in the HHHP from 2001 to 2024. WUE showed an overall upward trend across 78.53% of all pixels in the study domain. Specifically, 36.06% of the area exhibited significant growth, while 42.47% showed slight increases. These positive trends were mainly concentrated in the southwestern and northeastern regions of Shandong’s hilly areas, the Bohai Bay Area, the central North China Plain, and the northern Huang–Huai Plain. Conversely, regions experiencing slight or significant declines accounted for approximately 15.48% of the area, primarily located in the western and eastern North China Plain. GPP, T, and ET all showed increasing trends across over 90% of the study area, with proportions reaching 93.98%, 91.70%, and 91.32%, respectively. Significant increases were observed in 84.97%, 75.42%, and 69.57% of these areas, respectively. In contrast, the GPP/T ratio showed relatively lower growth rates, covering 25.91% of the total area. These increases were mainly distributed in the northern, western, and central parts of the study zone, with only 3.51% of the areas experiencing significant upward trends. The spatial distribution characteristics of the trends in T/ET and WUE were comparable, with 78.46% of the areas showing increasing trends. Among these, significant growth occurred in 22.65% of the regions, while slight increases accounted for 55.81%.

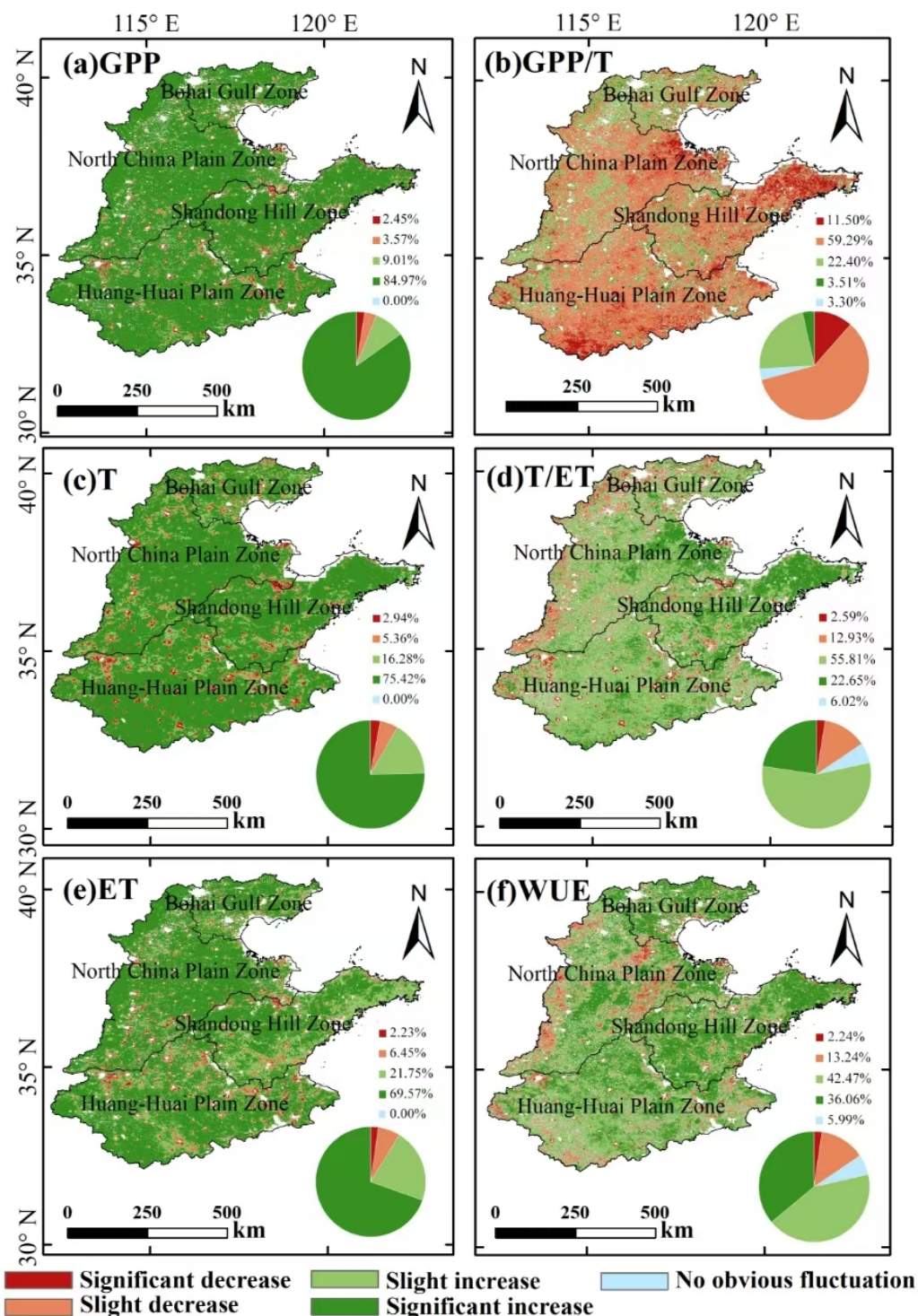


Figure 3. Trends of WUE, GPP, ET and their intermediate processes in the HHHP from 2001 to 2024. Panels (a–f) represent the spatial pattern of trend slopes for (a) GPP, (b) GPP/T, (c) T, (d) T/ET, (e) ET, and (f) WUE, respectively.

4.1.3. Time Variation Trend of WUE

The trends in WUE and its intermediate processes across the HHHP and its four subregions from 2001 to 2024 are presented in Figure 4. During the past 25 years, with the exception of the GPP/T, WUE, T/ET, GPP, ET, and T have all demonstrated an overall gradual upward trend. The WUE of the HHHP displayed an increasing trend at a rate of $0.004 \text{ g C m}^{-2} \text{ mm}^{-1} \text{ a}^{-1}$. Among the four subregions, the Shandong Hilly Region had the fastest increase rate in WUE ($0.006 \text{ g C m}^{-2} \text{ mm}^{-1} \text{ a}^{-1}$),

while the North China Plain Region had the slowest ($0.003 \text{ g C m}^{-2} \text{ mm}^{-1} \text{ y}^{-1}$). The GPP/T of the Huang–Huai Plain Zone demonstrated a downward trend at a rate of $-0.015 \text{ g C m}^{-2} \text{ mm}^{-1} \text{ a}^{-1}$, with the Shandong Hilly Region experiencing the fastest decline ($-0.029 \text{ g C m}^{-2} \text{ mm}^{-1} \text{ a}^{-1}$). The T/ET of the Huang–Huai Plain Zone showed an upward trend at a rate of $0.0049 \text{ mm mm}^{-1}$. The highest increase rate was observed in the North China Plain Region (0.005 mm mm^{-1}), followed by the Shandong Hilly Region, the Huang–Huai Plain Zone, and the Bohai Bay Region. The trends for GPP, ET, and T in the HHHP were $8.86 \text{ g C m}^{-2} \text{ y}^{-1} \text{ a}^{-1}$, $4.27 \text{ mm}^{-1} \text{ a}^{-1}$, and $5.54 \text{ mm}^{-1} \text{ a}^{-1}$, respectively.

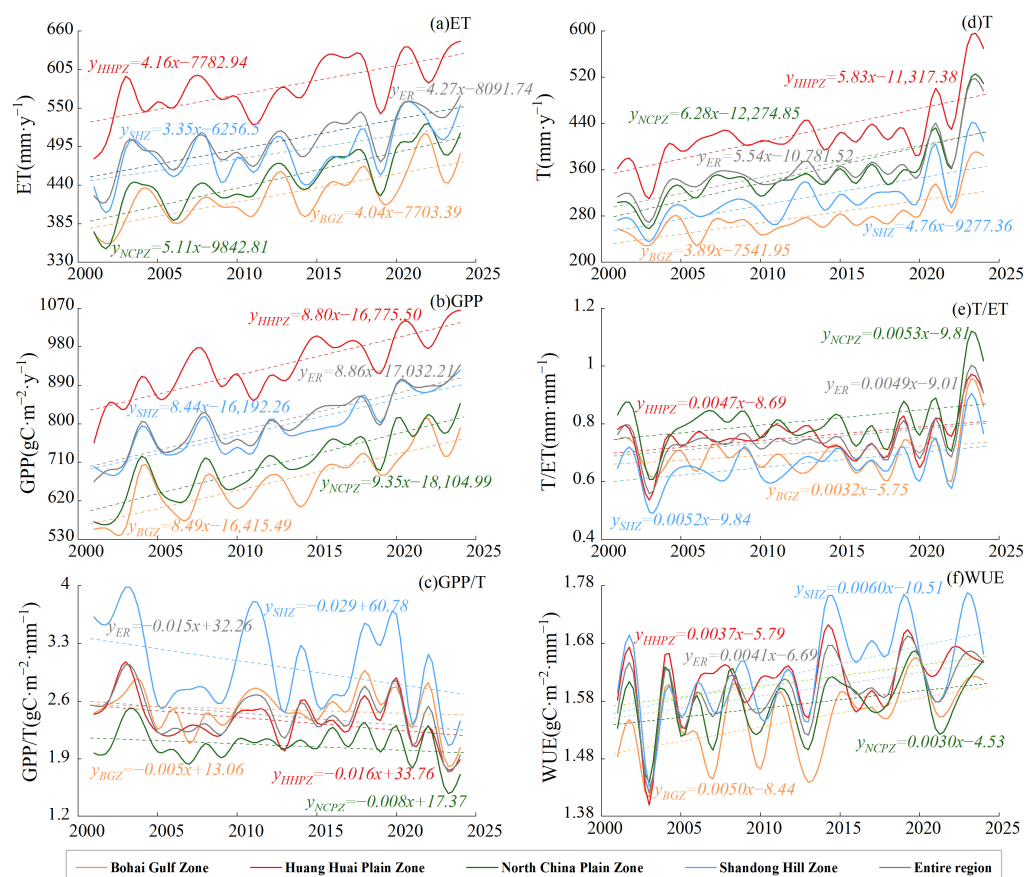


Figure 4. Trends of WUE, GPP, ET and their intermediate processes in the HHHP and its sub-regions from 2001 to 2024 ((a): interannual variation in ET; (b): interannual variation in GPP; (c): interannual variation in GPP/T; (d): interannual variation in T; (e): interannual variation in T/ET; (f): interannual variation in WUE).

4.2. Variation Trends of WUE Across Different Vegetation Types

Figure 5 illustrates the trends of WUE, GPP, ET, and their intermediate mechanisms among various vegetation types in the HHHP from 2001 to 2024. Notable differences were observed in the annual mean WUE values across different vegetation types. Ranked from highest to lowest, the values were as follows: shrublands (SHR) > woody savanna (WSA) > forest land (FOR) > savanna (SAV) > cropland (CRP) > farmland/natural vegetation patches (MOS) > grassland (GRS) > wetlands (WET). Specifically, SHR exhibited a WUE of $1.75 \text{ g C m}^{-2} \cdot \text{mm}^{-1}$, while wetlands showed a WUE of $1.34 \text{ g C m}^{-2} \cdot \text{mm}^{-1}$. The annual mean WUE values demonstrated significant interannual variations. Wetlands exhibited a declining trend, whereas other vegetation types showed increasing trends. Among them, cropland demonstrated the fastest growth rate in WUE ($0.0045 \text{ g C m}^{-2} \cdot \text{mm}^{-1} \text{ a}^{-1}$), while WSA had the slowest increase ($0.0014 \text{ g C m}^{-2} \cdot \text{mm}^{-1} \text{ a}^{-1}$). Wetlands exhibited the most pronounced fluctuations in the GPP/T ratio, showing an overall downward

trend. FOR recorded the highest T/ET value ($0.88 \text{ mm} \cdot \text{mm}^{-1}$). Wetlands demonstrated the fastest growth rate in T/ET ($0.0094 \text{ mm} \cdot \text{mm}^{-1} \cdot \text{a}^{-1}$), while WSA showed the most significant decline. ET exhibited a fluctuating upward trend across different vegetation types, with WSA showing the highest ET ($617.96 \text{ mm} \cdot \text{y}^{-1}$) values and the fastest growth rate ($9.73 \text{ mm} \cdot \text{y}^{-1} \cdot \text{a}^{-1}$) among all vegetation types. The growth pattern of GPP was consistent with the ET trends, as both FOR and WSA demonstrated higher GPP values than other vegetation types, with growth rates of $11.84 \text{ g C} \cdot \text{m}^{-2} \cdot \text{y}^{-1} \cdot \text{a}^{-1}$ and $16.58 \text{ g C} \cdot \text{m}^{-2} \cdot \text{y}^{-1} \cdot \text{a}^{-1}$, respectively. Additionally, the T in FOR and WSA was significantly higher than that in other vegetation types and showed an upward trend.

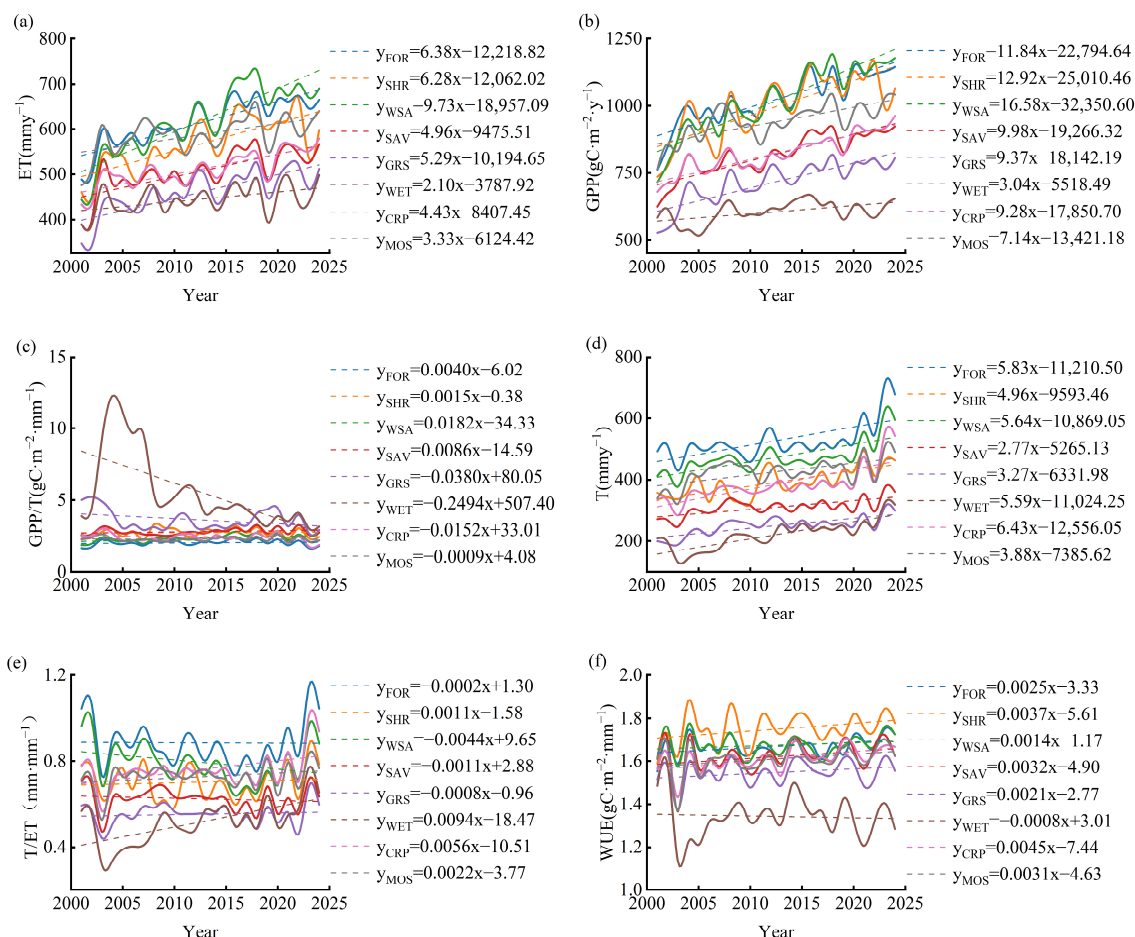


Figure 5. Variation trends of WUE, GPP, ET and their intermediate processes across different vegetation types in the HHHP from 2001 to 2024. Panels (a–f) show time series of (a) GPP, (b) GPP/T, (c) T, (d) T/ET, (e) ET, and (f) WUE for each vegetation type. Each subplot includes linear trend lines ($y = mx + b$) for all vegetation types over the 2001–2024 period.

4.3. Persistence and Temporal Stability of WUE

The spatial distribution patterns of WUE stability and sustainability in the HHHP are presented in Figure 6. In terms of stability (Figure 6a), WUE fluctuations are dominated by medium–low (56.97%) and low (29.64%) volatility regimes, which collectively account for 86.61% of the total study area. This suggests that interannual variations in WUE were relatively stable across most of the region. Areas with low volatility were mainly concentrated in the Huang–Huai Plain and the western Shandong hilly region, reflecting relatively stable hydrothermal conditions or more effective agricultural management practices that help mitigate interannual WUE fluctuations. In contrast, areas with medium–high (1.78%) and high (1.09%) volatility were limited in extent and sporadically distributed in coastal

tidal flats, wetlands, and regions with frequent land-use changes. These regions are likely influenced by extreme climatic events or anthropogenic disturbances, leading to greater interannual variability in WUE. Regarding historical persistence (Figure 6b), the potential continuation of WUE was dominated by persistent increases. Slight persistent increase and significant persistent increase accounted for 42.03% and 38.20%, respectively, totaling 80.23%. This indicates that the current increasing trend in WUE exhibits strong historical persistence across most areas, suggesting that this pattern may continue. These two categories extensively cover the central North China Plain, the Huang–Huai Plain, and most of the Shandong hilly region, representing the main areas of beneficial WUE development in the region. Conversely, slight persistent decrease and significant persistent decrease accounted for 12.77% and 2.37%, respectively, totaling 15.14%. These decreases were mainly observed in the northern North China Plain.

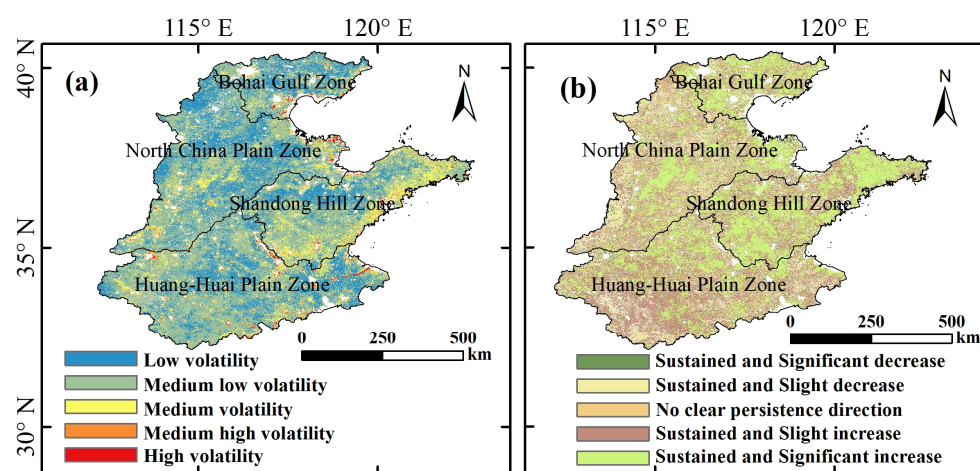


Figure 6. The spatial distributions of WUE stability and sustainability in the HHHP from 2001 to 2024. (a) WUE stability; (b) WUE sustainability.

4.4. Driving Mechanisms of WUE Temporal–Spatial Variations

4.4.1. Spatial Distribution of SHAP Values for the Impact of Driving Factors on WUE

Figure 7 illustrates the spatial distribution of SHAP values for factors influencing WUE in the HHHP region from 2001 to 2024. SHAP analysis indicates that NDVI is the strongest positive factor associated with WUE, accounting for 70.51% of the variation in WUE, followed by AI, which accounts for 60.43% of the variation in WUE (Table 3). The positive effects of NDVI were predominantly observed in the Huang–Huai Plain and North China Plain regions. Tem exerted the most widespread negative effect on WUE, impacting roughly 61.21% of the study area. This negative influence shows a clear intensification gradient from north to south, while localized positive effects are observed in the hilly regions of Shandong. Pre and drought index patterns displayed high similarity. Both factors had negative impacts in the North China Plain, while being associated with WUE enhancement in the Huang–Huai Plain. Pre contributed to 55.19% of the areas with positive influence. Significant negative effects of Pre were also observed in the southern Bohai Bay region. PET and Rhu showed positive associations with WUE, with coverage rates of 47.76% and 43.29%, respectively. These positive effects were primarily observed in the western North China Plain and eastern Bohai Bay regions. Coastal areas, however, showed pronounced negative impacts from PET. Overall, Tem remains the dominant limiting factor associated with WUE decline, while NDVI is the primary factor associated with WUE improvement. Among the other factors, PET and Rhu predominantly show negative associations, whereas Pre and AI show positive associations.

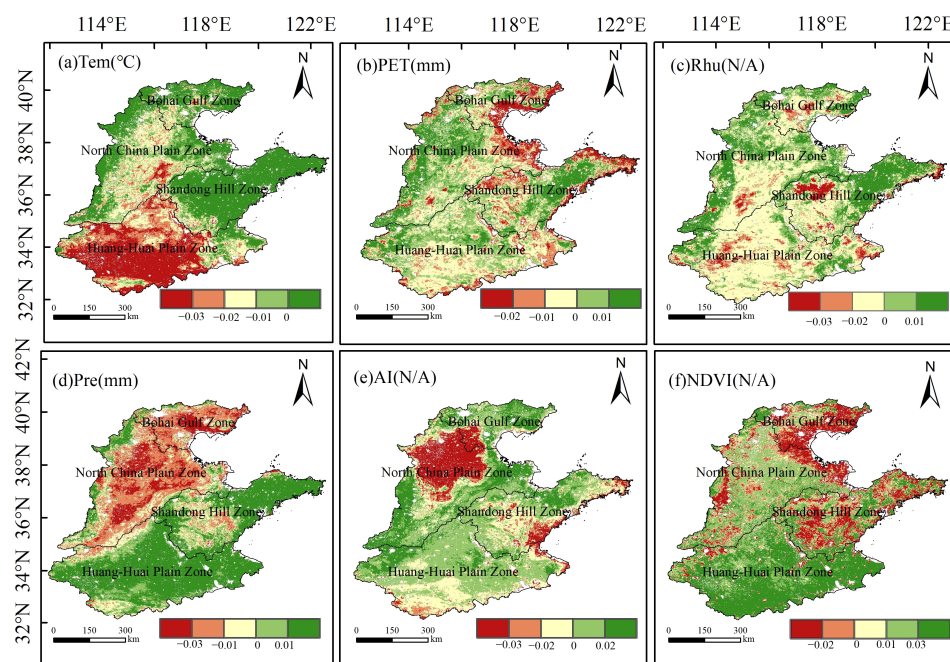


Figure 7. Spatial distribution of SHAP values for WUE driving factors in the HHHP from 2001 to 2024. Figures (a–f) show the spatial distributions of SHAP values for WUE in relation to Temp, PET, Rhu, Pre, AI, and NDVI, respectively.

Table 3. The positive and negative proportions of the impact of driving factors on WUE.

Impact Polarity	Temp	PET	Rhu	Pre	AI	NDVI
Negative value (%)	61.21	52.24	56.71	44.81	39.57	29.49
Positive value (%)	38.79	47.76	43.29	55.19	60.43	70.51

4.4.2. Summary Statistics of Driving Factors SHAP Values

Figure 8 displays the aggregated SHAP values of the factors influencing WUE in the HHHP. Based on the magnitude of their association with WUE, ranked from highest to lowest, the factors are NDVI, Temp, AI, Pre, Rhu, and PET. The SHAP dendrogram further elucidates the effects of these factors. High NDVI values are associated with positive SHAP coefficients, indicating that vegetation greening is the dominant factor associated with WUE improvement in the region. Similarly, elevated Pre values demonstrate positive SHAP effects, suggesting that increased Pre is associated with WUE enhancement. However, high Tem values are linked to negative SHAP coefficients, reflecting a strong negative association between heat stress and WUE. This phenomenon is consistent with the intensified ET and suppressed photosynthesis widely observed under regional warming and drought stress.

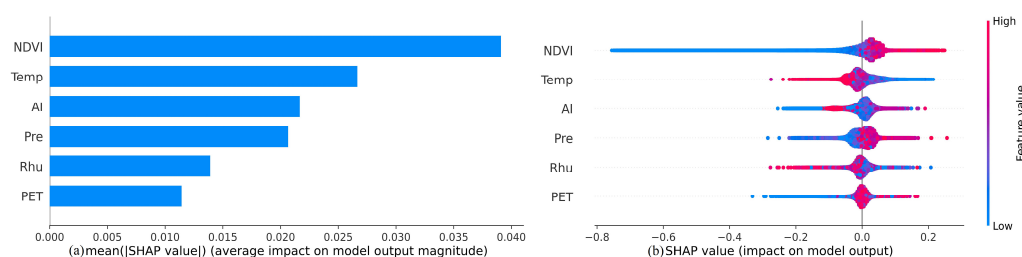


Figure 8. Summary statistics of SHAP values for WUE driving factors in the HHHP. Figure (a) represents the average absolute SHAP value of each driving factor, indicating the average impact magnitude on model outputs; Figure (b) shows the SHAP values of each driving factor, reflecting the direction and magnitude of their influence on model outputs.

4.4.3. Spatial Distribution of Dominant Factors in WUE Temporal–Spatial Variations

The results of the SHAP analysis for factors associated with WUE in the HHHP from 2001 to 2024 are presented in Figure 9. This section identifies the dominant associated factor for each pixel based on the maximum absolute SHAP value, which differs from the SHAP sign analysis in Section 4.4.1, which focuses on the direction (positive or negative) of each factor's contribution. The relationships between these factors and WUE exhibited significant spatial heterogeneity in both direction and intensity of contribution. Among the factors, NDVI had the highest median SHAP value, indicating its strongest driving effect on WUE. It dominated approximately 40.36% of the vegetation coverage area, primarily distributed in the western Shandong hilly region, as well as the eastern and southern Huang–Huai Plain region. Temp was the second most influential factor, exerting dominance over about 26.43% of the vegetation coverage area, mainly located in the central and western Shandong hilly region, as well as the central and southeastern Huang–Huai Plain region. AI and Pre served as secondary associated factors, with dominant effects on WUE in approximately 16.99% and 10.58% of the vegetation coverage area, respectively, with both factors predominantly observed in the North China Plain region. The dominant influence ranges of Rhu and PET were more limited, accounting for only about 4.03% and 1.62%, respectively, indicating their relatively limited overall importance for WUE.

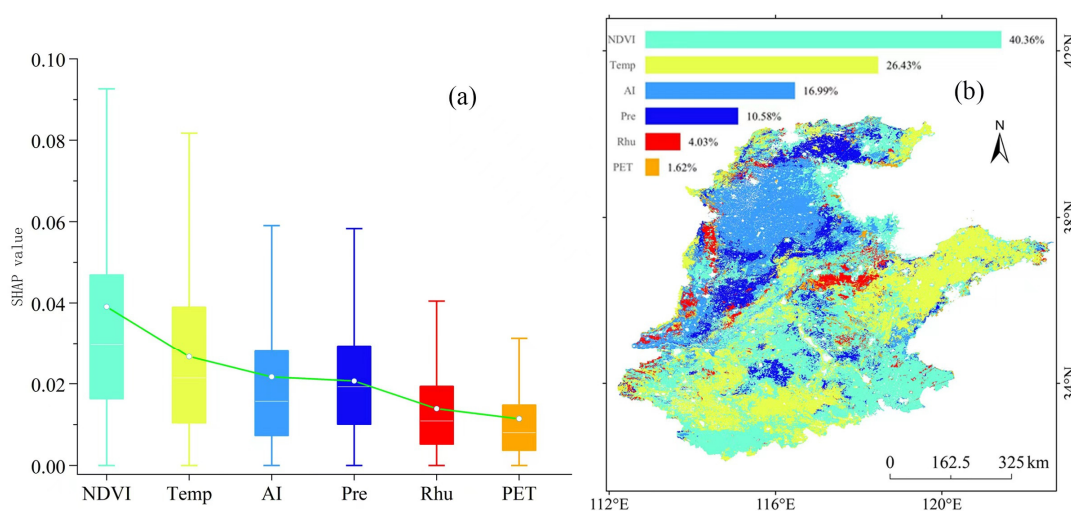


Figure 9. SHAP analysis results of WUE driving factors in the HHHP from 2001 to 2024. Figure (a): summary characteristics of absolute SHAP values; Figure (b): spatial distribution of absolute SHAP values for each driving factor.

5. Discussion

5.1. Spatial Patterns of WUE Across the HHHP

This study reveals the spatiotemporal dynamics of WUE within the HHHP ecosystem over the period 2001–2024, which does not fully align with the distribution of GPP and ET increasing from northwest to southeast. This indicates that WUE is not solely governed by GPP or ET alone; instead, it spatially reflects their proportional balance, confirming WUE's characteristic as a core indicator for carbon–water coupling processes [38]. The overall trend in WUE identified in this study shows a significant increase, accounting for 78.53% of the study area, which is consistent with rising trends observed globally and in many regions of China [39–41]. To place the research findings in a specific context, we compared the WUE results from this study with those from previous studies in the HHHP region and neighboring areas. The multi-year average WUE of farmland in this study was generally consistent with field estimates from the HHHP region, where the WUE of winter wheat

under optimized cropping patterns ranged from 2.16 to 2.26 kg·m⁻³ [42]. The multi-year average WUE for the entire North China Plain ecosystem was 0.74 g C·m⁻², a value lower than the estimates in this study, which may be because their study covered a broader range of ecosystem types, whereas this study focused on areas with higher-productivity vegetation cover [43]. On the Loess Plateau, WUE increased significantly between 1985 and 2015, which is consistent with the upward trend observed in this study [44], although the magnitude of the increase differs due to variations in the study period, spatial resolution, and the definition of WUE. These comparisons reveal significant heterogeneity in WUE values and trend rates across different regions and study periods, underscoring the importance of region-specific assessments for understanding carbon–water coupling dynamics. However, it is noteworthy that significant heterogeneity exists within the HHHP dataset. The rate of WUE increase was highest in the Shandong hilly region (0.006 yr⁻¹) and lowest in the North China Plain (0.003 yr⁻¹), highlighting the necessity for refined assessments at regional scales, as large-scale trends may mask differences in responses to climate and human activities across subregions [15,45].

Although GPP, ET, and T exhibited widespread increasing trends (area coverage > 90%), the intermediate processes connecting them showed divergent patterns. The GPP/T declined or showed slight increases in most regions (approximately 74%), while T/ET followed a similar trend to WUE, predominantly showing an upward trajectory (78.46%). These findings suggest that the WUE improvement across the HHHP ecosystems over the 24-year period was primarily driven not by enhanced carbon sequestration capacity per unit of T, but rather by an increased proportion of T in total ET, indicating that more water was dissipated through physiological processes (T) rather than physical processes (evaporation) within vegetation [7]. This aligns with recent studies based on process chain frameworks, which have identified T/ET as a key intermediate process in WUE variation within arid and semi-arid ecosystems [9]. While GPP experienced rapid growth, T increased at an even faster rate or was influenced by stress factors such as high T_{em}, leading to a general decline in the water cost-effectiveness ratio of photosynthesis and the GPP/T ratio [46]. Temporally, the upward trends in WUE, T/ET, GPP, ET, and T, coupled with the downward trend in GPP/T, further support this inference.

5.2. Spatiotemporal Changes in WUE Across the HHHP

This study confirms that ecosystem WUE exhibits significant dependence on vegetation type. In HHHP, the multi-year average WUE ranking across different vegetation types was as follows: SHR > WSA > FOR > SAV > CRP > MOS > GRS > WET. This ranking shares similarities with global patterns of WUE variations among ecosystems while also reflecting regional specificity [23,47,48]. SHR exhibited the highest WUE and the highest GPP/T ratio, while their T/ET ratio was comparable to that of other vegetation types. This suggests that the high WUE of SHR is more closely associated with GPP/T. Furthermore, SHRs are primarily distributed in the hilly regions of Shandong, where NDVI values have risen significantly; our SHAP analysis further indicates that NDVI is a major positive contributor to WUE in this region. These patterns are consistent with the view that the high WUE of SHR may be attributed to vegetation greening under mild to hot conditions. This is primarily due to their unique structural and physiological adaptations to arid and semi-arid environments; such SHRs typically possess deep root systems capable of efficiently utilizing water reserves in deep soil layers, thereby maintaining sustained physiological activity during water stress [49]. In the HHHP region, areas covered by SHRs feature undulating terrain, limited soil water-holding capacity and deep groundwater tables, which collectively create a relatively arid microenvironment. Therefore, the higher WUE observed in shrub communities may reflect their adaptive response to local water scarcity, which is consistent

with the findings of previous studies. Additionally, their high LAI allows for efficient capture of light energy, while water-saving physiological mechanisms, such as regulated stomatal conductance, minimize water loss [50]. However, since traits such as root distribution and stomatal conductance were not measured, the exact mechanism remains to be verified by future research. This combination of “high photosynthetic potential and low T water consumption” enables shrubs to sequester more carbon per unit of water consumed, resulting in their superior WUE. In contrast, wetlands exhibited the lowest WUE, owing to their unique anaerobic, water-saturated habitats. Persistent flooding leads to soil anoxia, severely inhibiting root aerobic respiration and activity. This, in turn, limits water and nutrient uptake as well as the distribution of photosynthetic products to above-ground tissues, directly diminishing vegetation’s photosynthetic capacity [51].

WUE trends differed considerably among vegetation types. While wetlands exhibited a declining WUE, all other types showed increasing trends, with agricultural land demonstrating the most rapid growth. This improvement can be attributed to continuous crop variety optimization, advanced irrigation management practices, and enhanced CO₂ fertilization effects driven by increased nitrogen deposition. These measures have substantially improved production capacity and resource utilization efficiency in farmland ecosystems [22,24,52]. Conversely, the declining WUE in wetlands, coupled with a marked reduction in their gross primary production per unit area (GPP/T), indicates heightened vulnerability to climate change or human disturbances, as well as rising water costs associated with carbon sequestration processes [53]. Furthermore, FOR and WSA exhibited the highest absolute values and growth rates of GPP and T, yet their WUE was not the highest, and the growth in GPP/T was not significant. This indicates that while these woody vegetation types excel in total carbon sequestration and water consumption, their “marginal benefit” of water use—that is, the additional carbon sequestration per unit of water consumed—may be approaching saturation or constrained by other factors [54]. This finding aligns with previous studies, revealing relatively low CUE in forest ecosystems and their complex responses to climate change [55,56].

5.3. Impact of Driving Factors on WUE in the HHHP

This study reveals the spatial heterogeneity in the dominant drivers influencing WUE within the HHHP ecosystem. NDVI showed the strongest association with WUE, with positive contributions across 70.51% of the region and dominant explanatory power in 40.36% of vegetated areas. This finding directly supports the notion that increased vegetation greenness or coverage represents the core biological pathway for enhancing carbon–water coupling efficiency in HHHP ecosystems, primarily through enhanced photosynthesis (GPP), consistent with findings from numerous global studies [26,57,58]. Tem was identified as the primary limiting factor, exhibiting an adverse effect on WUE in 61.21% of the regions and playing a dominant role in 26.43% of them. The negative SHAP value associated with high Tems demonstrates that under the warming and drying conditions of the HHHP, rising Tems intensify atmospheric ET demand, leading to ET increases that outpace GPP growth or trigger photosynthetic stress such as stomatal closure, thereby suppressing WUE [46]. Interestingly, Temp exhibited a positive effect in the hilly regions of Shandong, revealing the regional context-dependent nature of driver factors’ influence, which is associated with local specific moisture conditions, vegetation types, or topography that mitigate heat stress [59].

Both Pre and the aridity index predominantly exhibit positive effects on WUE, with positive contributions in 55.19% and 60.43% of the region, respectively. This reflects the dual role of water factors: moderate Pre increases alleviate drought stress and enhance WUE, while higher aridity index values may promote WUE through conservative water-use

strategies such as stomatal regulation. The coexistence of positive Pre and aridity index effects suggests a nonlinear, context-dependent relationship: in wetter areas, additional Pre relieves moisture stress, whereas in drier areas, higher aridity index favors water-saving mechanisms. However, in flat terrain with inadequate drainage, excessive Pre can reduce WUE via increased non-productive evaporation or waterlogging stress [60]. As an integrated indicator of aridity that combines Pre and PET, higher aridity index values indicate drier conditions. Its overall positive effect on WUE suggests that moderately drier conditions—or more precisely, a relative balance favoring evaporative demand over precipitation—may enhance WUE by limiting non-productive water loss and promoting more efficient water use by vegetation [61]. In contrast, PET and Rhu exerted relatively weak effects, with large spatial heterogeneity in both the sign and magnitude of their impacts [3]. This study quantified the relative importance of WUE driving factors in the HHHP region ($\text{NDVI} > \text{Temp} > \text{AI} > \text{Pre} > \text{Rhu} > \text{PET}$) and their spatial heterogeneity patterns, which are consistent with global analyses [39,47]. These findings indicate that the driving mechanism of WUE results from the nonlinear interactions of multiple factors, including climate, vegetation, topography, and human activities, and exhibits high spatial heterogeneity.

5.4. Practical Significance and Limitations of the Research Findings

Despite its contributions, this study has several limitations. First, the remote sensing data products employed for GPP and ET inherently carry uncertainties. Although these data have been validated and are widely applied, their accuracy may be compromised over complex land surfaces. To further improve the reliability of input data, future research could integrate multi-source fusion data products such as GloFlux, or adopt novel modeling frameworks represented by FLAML-LUE [56,62]. Second, this study's examination of the drivers behind WUE is mainly based on statistical correlations. While SHAP values provide strong interpretability, the causally ecological and physiological processes underlying these relationships still require validation through process-based models or controlled experiments. Third, this study employed XGBoost as the primary machine learning model for driver analysis without conducting a systematic comparison with other models. To further confirm the advantages and robustness of XGBoost, future research should compare its performance with other commonly used machine learning models, such as Random Forest, LightGBM, CatBoost, or traditional multiple regression methods, under the same input data and evaluation framework. Such comparative studies would help verify the reliability of the SHAP interpretation results and provide a more comprehensive understanding of model-driven factor analysis. Future investigations could focus on the following directions: First, the analysis should be extended to future scenarios by utilizing climate model data from the CMIP6 and ecosystem models to forecast the development of WUE in the HHHP under different Shared Socio-Economic Pathways (SSPs), thus evaluating the long-term effects of climate change and anthropogenic activities. Second, the quantification of human management factors should be refined by incorporating specific agricultural management data, such as fertilization practices, irrigation systems, and cultivation methods, to measure their contributions to WUE and related processes (GPP/T , T/ET), aligning with research aimed at improving low-carbon land use efficiency through optimized management strategies. Third, studies on carbon–water coupling synergies and trade-offs should be expanded to identify regions and relationships where WUE and CUE exhibit coordinated changes under HHHP conditions, providing an integrated perspective for achieving the dual objectives of carbon neutrality and water security at the regional level.

6. Conclusions

Drawing upon multi-source remote sensing data spanning from 2001 to 2024, this study systematically investigated the spatiotemporal dynamics and driving mechanisms of ecosystem WUE in the HHHP. The key findings are as follows: (1) WUE showed a predominantly increasing trend across 78.53% of the study area, with notable increases (36.06%) concentrated in the southwestern Shandong hilly region and the central North China Plain. High WUE values ($1.68\text{--}1.74\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$) were observed in the eastern Shandong hills and the southwestern North China Plain, while low values ($1.50\text{--}1.56\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$) were found in the northern North China Plain and the southeastern Bohai Bay area. (2) Among different vegetation types, shrubland exhibited the highest multi-year mean WUE ($1.75\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$), whereas wetland had the lowest ($1.34\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}$). Cropland showed the most rapid increase in WUE ($0.0045\text{ g C}\cdot\text{m}^{-2}\cdot\text{mm}^{-1}\cdot\text{a}^{-1}$), while wetland displayed a decreasing trend. (3) The HHHP ecosystem demonstrated a favorable pattern of low volatility and strong sustainability, with stable interannual WUE and a projected continuous increase across most areas in the future. (4) NDVI produced positive WUE responses over 70.51% of the study area and served as the dominant driver for 40.36% of vegetated pixels, whereas Tem acted as the primary negative constraint, suppressing WUE over 61.21% of the region. Pre and AI played secondary roles, with positive effects mainly in the Huang–Huai Plain and negative effects in the North China Plain. These results offer key scientific support for coordinated regional water–carbon management and targeted ecological conservation across the HHHP.

Author Contributions: Y.L. (Yan Li): Investigation, resources, data curation, writing—original draft, formal analysis, methodology. F.Y.: Data curation, conceptualization, visualization. Y.L. (Yuhong Liu): Resources, formal analysis, validation. G.L.: Writing—original draft, formal analysis, resources. Z.Y.: Resources, methodology, writing—review & editing. Z.S.: Software, formal analysis. F.W.: Data curation, visualization. All authors have read and agreed to the published version of the manuscript.

Funding: This study was supported by the Research Project of Humanities and Social Sciences in Universities of Henan Province (2027-ZZJH-074, 2021-ZDJH-047); the Henan Provincial Key Science and Technology Research Program (262102110354); the Science and Technology Research and Development Program of Henan Province (262102110336); the Joint Fund of Science and Technology Research and Development Program of Henan Province (252103810058, 252103810083); Development of Land Rehabilitation Database System of Henan University of Urban Construction (990-K-H2023323); and the Xinxiang City Social Science Federation Research Project (SKL-2026-0060).

Data Availability Statement: The datasets used and/or analyzed in this study are available from the corresponding author upon reasonable request.

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

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