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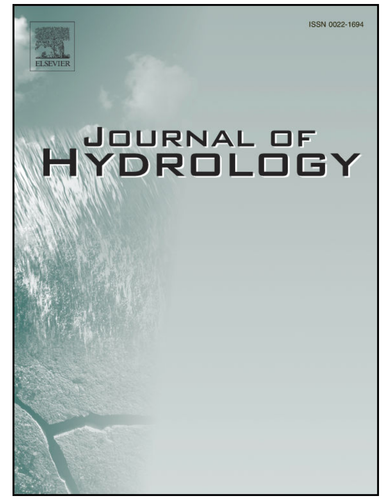

Research papers

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Untangling the coupling effect of water quality and quantity on lake algal blooms in Lake Hulun from a dual perspective of remote sensing and sediment cores

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Untangling the coupling effect of water quality and quantity on lake algal blooms in Lake Hulun from a dual perspective of remote sensing and sediment cores

a) Highlights

Dual-scale view of algal blooms: remote sensing image and sediment core sample.

Utilization of multiple analysis methods, including Copula, GAM, and SEM analysis.

The nonlinear water quality and quantity variation exhibited a turning point in water level changes at 543 meters.

Through indirect coupling effects, water level changes dominate water quality shifts, algal blooms, and diatom community variations.

(ii) Abstract

Algal blooms and sediment diatoms are crucial indicators of lake water ecology, influenced by water quantity and quality. However, the coupled effects of water quality and quantity changes on algal blooms are still unclear, especially for lakes in cold and arid regions. This study assessed the long-term variations in algal blooms in Hulun Lake using a novel approach combining remote sensing and sediment core samples for diatom analysis. Two mutation points from the structural change test were identified in approximately 2000 and 2010 for algal bloom area (MBE) and sediment diatom richness, indicating asynchronous algal blooms. A structural equation model (SEM) demonstrated that water level (WL) changes were the dominant influencing factor, co-driving the variations in algal blooms and sediment diatoms in conjunction with total nitrogen (TN), total phosphorus (TP), and chemical oxygen demand (COD). The results revealed nonlinear relationships between the lake WL, TN, Chla, and COD. The water level of 543 m emerged as a critical threshold affecting the relationship between water quality and quantity. Distinct differences in this relationship were observed when water levels were above or below this threshold. These variations became particularly pronounced during periods of high and low water levels. The results provide novel insights into the dynamics of algal blooms and can further support lake ecosystem conservation and management.

Keywords: Algal blooms, water quality, water quantity, coupling effects, Hulun Lake

1. Introduction

Algal blooms have become one of lakes' most critical environmental issues worldwide. Recent research highlights a significant increase in algal blooms across global freshwater lakes, with marked rises, particularly in Asia and Africa over the last four decades (Hallegraeff et al.,2021; Hou et al., 2022; Sha et al., 2021). This trend is further complicated by the interplay between deteriorating water quality and shifting hydrological conditions (Ho et al., 2021; Van Vliet et al.,2023); in places like China, worsening water quality not only causes eutrophication but also leads to ecological degradation and biodiversity loss. Therefore, implementing more effective measures to control eutrophication and restore aquatic ecosystems is urgently needed (Babamiri and Marofi, 2021; Yang et al., 2021; Zhang et al., 2022). Water quantity and quality management have been recognized as crucial factors for controlling algal blooms, but their coupling effects are still unclear (Cui et al., 2021). Investigating the impact of water quality and quantity on algal blooms while considering the relationship between water quality and water quantity may help to elucidate the mechanisms behind algal blooms further and provide essential insights for the coordinated management of lakes.

Sediment cores as biomarkers have been widely used in hydrogeological research to study the temporal changes in biological communities (Capo et al., 2019; Li et al., 2019; Naeher et al., 2012). Among these biomarkers, diatoms are suitable for studying the long-term dynamics of algal ecosystems due to their broad habitat distribution, sensitivity to environmental changes, and indicative influence on lake nutrition, hydrology, and aquatic vegetation (Chen et al., 2021; Moser, 2004; Wang et al., 2012). However, collecting sediment samples requires field sampling and laboratory analysis, which is costly and time-consuming (Zhang et al., 2021b). In contrast, remote sensing provides an alternative means. Due to the spatial and temporal coverage of remote sensing images, remote sensing techniques can be used to monitor the dynamics of algae blooms (Zhang et al., 2021a) over a large extent and an extended period. However, the quality of remote sensing images is influenced by weather conditions, which could introduce further errors in the estimates of algal blooms. Remote sensing monitoring focuses on identifying algal blooms using specific spectral information. In contrast, the study of diatoms in sediments focuses on analyzing ecological characteristics such as the abundance and community structure of diatoms. Sediment analysis provides localized, detailed information about specific sites and requires physical sampling and laboratory analysis. It allows for identifying specific algal taxa and reconstructing past environmental conditions and historical algal blooms extending back decades or even centuries. Contrastingly, remote sensing data provides sizeable spatial coverage and facilitates temporal analysis of algal bloom dynamics but may be affected by cloud cover and have limitations in distinguishing between algal types. By integrating these two approaches, researchers can overcome the limitations of each method alone, providing a more nuanced and complete picture of algal bloom dynamics at different scales (Fig. 1). Few studies have combined the two approaches to investigate the ecological shifts within aquatic ecosystems.

Climate change impacts algal blooms directly by altering wind patterns and light irradiance, which are essential for bloom development (Fang et al., 2018; Thomas et al., 2017). Concurrently, human activities, including water management projects and overfishing, indirectly affect algal growth by modifying ecological balances and nutrient dynamics (Chen et al., 2021). Simultaneously, the impact of climate change and human activities on water quality and quantity is quite significant. The effects of climate change on water volume and quality are primarily manifested through alterations in precipitation, evaporation, and temperature changes. Meanwhile, human activities, such as water diversion projects and river flows, can introduce nutrient inputs into lakes, altering water quality and quantity. Consequently, these two impacts influence water quality and quantity through biogeochemical processes and ecosystem hydrodynamics, collectively affecting algal blooms (Zhang et al., 2022). However, the interplay between hydrological conditions and water quality, significantly influenced by climate change and human activities, plays a decisive role in developing algal blooms in lakes (Liu et al., 2022). The dual influence of water quality and quantity has been identified as the main driving force (Zuo et al., 2019). The close interaction between water quality and quantity inevitably leads to changes in biogeochemical and physical processes in the water body and sediments (Fig. 1), which may trigger the release of buried nutrients in sediments and algal blooms, as well as shifts in biological communities (Yang et al., 2021; Chen et al., 2020). However, existing studies mostly treated lake water quantity and water quality as independent variables without considering the interplay between water quantity and water quality (pathway 2 in Fig. 1) and overlooked their combined effects (pathway 1 in Fig. 1) (Zhang et al., 2019; Yan et al., 2022). Therefore, investigating the coupling effect of water quality and quantity on algal blooms is crucial.

To reveal the dynamic mechanism of algal blooms requires further study of the response relationship between water quality and water quantity. Previous works on lake water quantity and quality have mostly adopted two approaches. The first is based on mechanistic models. For example, Alamdari et al. (2022) assessed the impact of water quality and quantity on a watershed in northern Virginia by combining watershed hydrological models with reservoir water quality models. Yet, the mechanistic models require extensive data and calibration efforts. Another approach relies on statistical ones. This approach has advantages when data is limited (Atique & Attoh-Okine, 2016). For example, Zang et al. (2022) analyzed the joint probability distribution of discharge and TN/TP concentrations using the Frank copula function and identified quantitative management intervals. The Gaussian mixture model was introduced into their copula models to adaptively describe the joint effects of water quantity and water quality indicators for assessing the eutrophication risk. Copula functions have advantages in characterizing marginal distributions of different environmental parameters, but they have difficulties dealing with nonlinearity or threshold effects (Zhang et al., 2020; Li et al., 2023). Combining other models with the Copula approach, such as generalized additive models (GAM), may offer a more comprehensive understanding of the dynamic changes between water quality parameters and water levels and, consequently, support effective lake environment protection.

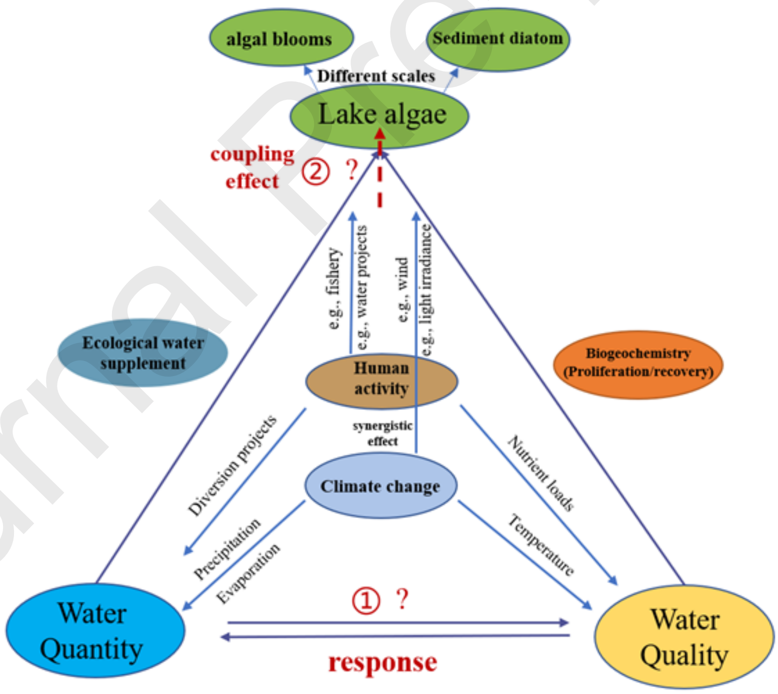

Fig. 1. Hypothesis of the role of water quantity and water quality in jointly controlling algal blooms and diatoms under various climatological and hydrological forcings. Sediment diatoms can be identified with sediment core samples, and algal blooms can be identified with remote sensing images.

Hulun Lake, the largest lake in northern China, has experienced remarkable economic growth, but the population expansion has continuously declined. Since the early 1990s, algal blooms have occurred several times that have jeopardized the local ecosystem of the lake (Fang et al., 2018). Despite decades of restoration efforts, the threat of algal blooms remains a concern (Chen et al., 2021). Taking Hulun Lake as an example, in this work, we hypothesized that the coupling of water quality and quantity primarily influenced algal blooms. Specifically, water quantity affects water quality and drives algal blooms via the coupling effect. Thus, the objectives of this study were as follows: (1) to characterize the variations in algal blooms in Hulun Lake using sediment diatoms and remote sensing data; (2) to quantify the impact and driving mechanisms of the coupled changes in water quality and quantity on algal blooms; and (3) to illustrate the response relationships between the water quality and quantity in Hulun Lake and identify key response factors. This work aimed to investigate the impact of coupled water quality and quantity variations on algal blooms and explore potential mechanisms. The results can contribute to implementing pollution control strategies and restoring aquatic ecosystems in cold and arid regional lakes.

(iii) 2. Materials and Methods

a) 2.1 Study Area

Hulun Lake (48°30′40″~49°20′40″N, 117°00′10″~117°41′40″E) is the fifth largest freshwater lake in China. It is located in the northern Inner Mongolia Autonomous Region, which is a cold and arid climate region. The lake has an area of 2339 km^2 with an average water depth of 5-6 m and a maximum depth of approximately 8 m. The two main water inflows are the Krulen and Urshen Rivers, respectively. In 2000, the lake level dropped sharply due to reduced precipitation, severe warming, and drying in the basin. Under these conditions, Hulun Lake became an endorheic lake. Water and pollution entering the lake have no way out. The eutrophication level has risen to an alarming level. In recent years, the local government has taken many measures, such as ecological water replenishment via water diversions, to restore the lake storage and improve the water quality. Although they have successfully restored the water level up to ~543 m above sea level, the lake's water quality remains poor and at risk of algal blooms.

b) 2.2 Datasets

In situ water quality data were obtained from field surveys from August 2006 to August 2019 at 13 water sampling sites (located in the western, middle, and eastern sections of the lake; Liang et al. (2016) and Yu et al. (2021)) (Fig. 2). The water quality parameters include pH, Secchi depth (SD, cm), dissolved oxygen (DO, mg/L), nutrient concentrations (i.e., TN and TP, μg/L), chlorophyll a (Chl a, μg/L), chemical oxygen demand (COD_{cr}). Lake surface water temperature (LSWT) was extracted from MOD11A2 remote-sensing images with 8-day and 1-km resolution. Correspondingly, the primary rivers that feed into Hulun Lake are the Kherlen River, Urson River, and Hailaer River. Data concerning river TN and TP levels were sourced from Yu et al. (2021), Pang et al. (2019), and research reports.

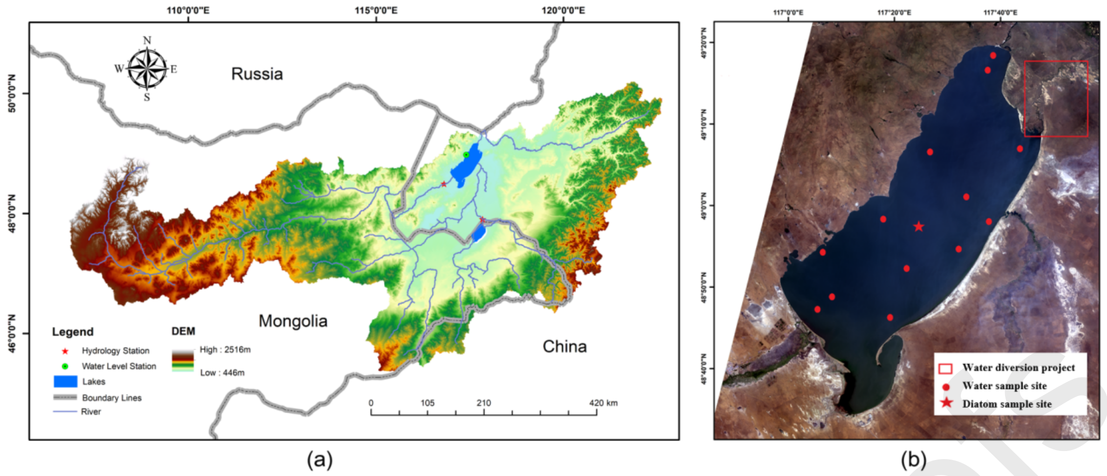

Fig. 2. Location of the study area. (a) The geographical location and elevation of the study area; (b) the location of the water diversion project and the distribution of field points.

i. 2.2.1 Sediment diatom counts with sediment cores

A gravity sampler collected sediment cores (approximately 30-40 cm long) from the lake. The sediment cores were then subsampled every 1 centimeter, frozen, and stored at -20 °C. The subsamples were pretreated for diatom analysis (Battarbee et al., 2001). The pretreated diatom concentrates were dropped onto glass slides. Naphrax® gum was then used to make slides after completely dried concentrates. The diatoms were counted under a 1000x oil microscope (Leica DM2500) according to the classification system of Krammer et al. (1991). The diatom count of each sample was limited to 400-450 grains, and the number of diatoms per gram of dry sediment was denoted as the diatom density (DD, 10^4 ind/g) (Matthews and Shakesby, 2004). The Margalef diversity index was used to represent the species richness of the diatoms, calculated as follows:

$$\mathrm{MD} = (\mathrm{S} - 1)/\ln \mathrm{N} \qquad (1)$$

Where MD represents the Margalef diversity index, S is the number of algae types, and N is the total diatom counts.

ii. 2.2.2 Algal bloom detection with remote sensing

We selected the Hou et al. (2022) algorithm for its pioneering use of the CIE color system in algal bloom detection, chosen for its precision and broad applicability across various lake environments. Compared to other methods for detecting algal blooms, the advantage of the CIE method is its ability to quantify and define colors using a two-dimensional CIE xy chromaticity diagram. This method allows for the numerical specification of colors based on human perceptibility using the visible spectrum. It has been confirmed this that algorithm is both reliable and accurate for Lake Hulun (Wang et al., 2023). This prior validation supports our utilization of the algorithm in our study, ensuring that our methodology is appropriate and scientifically robust for estimating algal bloom distribution in this particular environment. Remote sensing images from Landsat 5, 7 and 8 were obtained from the Google Earth Engine platform. For each pixel, we recorded the number of times that the pixel was classified as having an algal bloom event (denoted as N_{bloom}) and the number of valid Landsat observations (N_{valid}) that were not cloud-shadowed. We then calculated the maximum bloom extent (MBE) and the bloom occurrence (BO). The MBE represents the total area of pixels where algal blooms were detected at least once. The BO was estimated by normalizing N_{bloom} against N_{valid} and represents the proportion of Landsat observations during which an algal bloom was recorded.

$$BO = N_{bloom} / N_{valid} \tag{2}$$

Our dual-perspective approach, combining remote sensing for monitoring blue-green algae and sediment core analysis focusing on diatoms, is designed not only to leverage the strengths of each method but also addresses the limitations of remote sensing, such as variable image quality and seasonal discrepancies. Together, these methods provide a comprehensive understanding of algal bloom dynamics. Diatoms are well-known for their sensitivity to changes in water quality and have been widely used as bioindicators for historical environmental reconstructions. Their siliceous frustules preserve well in sediments, allowing for a detailed reconstruction of past water quality conditions (Wang et al., 2012). Preserving blue-green algae in sediment cores can be less reliable than diatoms, as cyanobacterial remains are more prone to decomposition (Ding et al., 2021). This can introduce biases or uncertainties in reconstructing past algal bloom events based solely on blue-green algae. Preliminary reviews of existing literature and studies on Hulun Lake suggested that diatoms provide a consistent and reliable proxy for historical water quantity assessments in this particular lake environment (Xue et al., 2003).

c) 2.3 Data analysis

In this study, we systematically integrate Structural Equation Modeling (SEM), Copula functions, and Generalized Additive Models (GAM) to intricately examine the roles of water quality and quantity in influencing algal bloom dynamics. SEM is initially applied to map the intricate relationships between water quality, quantity, and algal blooms. This approach allows us to understand water parameters' direct and indirect effects on algal blooms, establishing a structural framework for our analysis. However, SEM might not adequately address the complex, nonlinear dependencies between water quality and quantity. To bridge this gap, we introduce Copula functions. This method enhances the analysis by modeling the joint distribution of water quality and quantity, thereby uncovering the nuanced dependencies that SEM overlooks. This step allows us to comprehend better how variations in water quality and quantity jointly contribute to algal bloom conditions. To extend the analysis further, GAM is employed to dissect the nonlinear relationships between water quality and quantity, offering a more granular view of their interaction. Unlike SEM, GAM provides the flexibility to accurately model these intricate dynamics without predefining a specific relationship form, thus complementing our initial findings from SEM and the depth provided by Copula functions. Collectively, these methods constitute a robust analytical framework, each contributing uniquely to unraveling the complex interplay between water quality, quantity, and algal blooms. By employing SEM for structural analysis, Copula functions for dependency modeling, and

GAM for nonlinear exploration, we can better understand how water quality and quantity influence algal bloom dynamics.

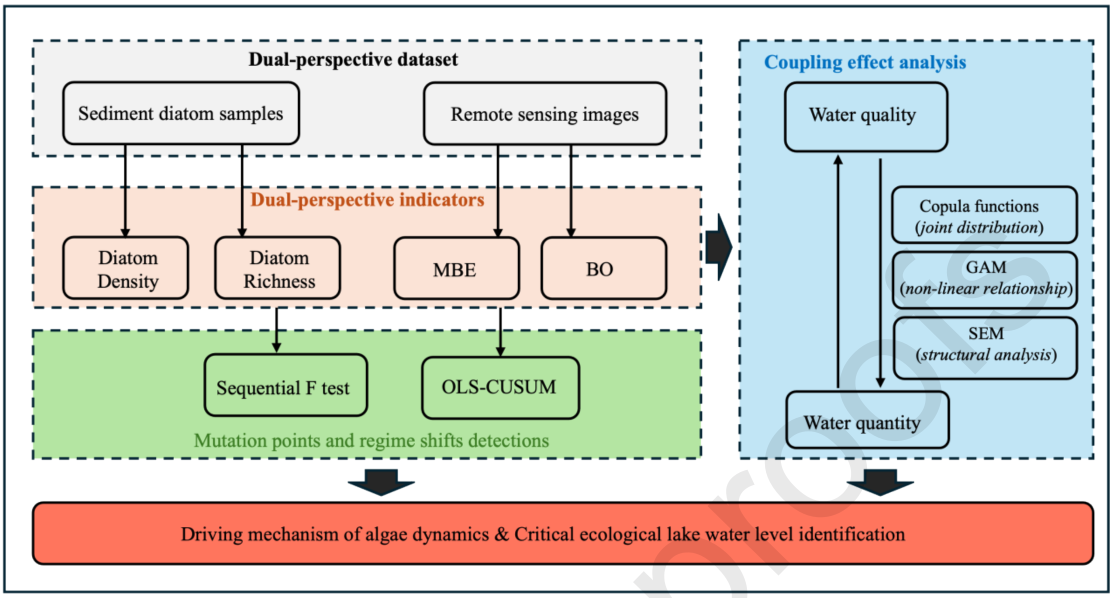

Fig. 3. Flowchart for the overall methodology.

i. 2.3.1 Mutation points and regime shifts detections

Detecting potential structural changes in data sequences has many applications in analyzing algal ecosystems. The Sequential F Test is a statistical method to detect breakpoints in time series data. It works by assuming that the data is continuous up to a certain point and then checking to see if a significant change occurred after that point (Kong et al., 2017). Sequential F test and breakpoint function analyses were used to estimate breakpoints by minimizing the residual sum of squares and Bayesian information criterion (BIC). In addition, ordinary least square cumulative sum (OLS-CUSUM) is a method for monitoring and analyzing potential structural changes in time series data. This study used the experience of empirical fluctuation processes cumulative sum based on ordinary least square residuals in OLS-CUSUM to analyze whether algal ecosystems undergo steady-state transformation (Brown et al., 1975). According to the theory of state transformation, for lake ecosystems that have undergone such a transformation, reducing external pressures to levels before the transformation does not revert the ecosystem to its original state along its previous developmental trajectory (Scheffer & Jeppesen, 2007). Steady-state transformations lie in their ability to indicate critical thresholds or tipping points beyond which ecosystems may not recover to their original state, thereby informing conservation strategies and management practices aimed at preserving ecological balance (Wang et al., 2012). This concept is widely applied in environmental science to understand the resilience of aquatic ecosystems to eutrophication (Sarkodie & Adams, 2018).

ii. 2.3.2 Structural equation modeling

Structural Equation Modeling (SEM) is a potent statistical methodology capable of precisely quantifying the cumulative impact of numerous influencing factors on target variables.

SEM offers a means to comprehensively analyze the intricate interplay between various factors and their collective influence on specific outcomes (Huang et al., 2023). SEMs were used to evaluate the impact of water quality and quantity on lake algal blooms and sediment diatoms. A maximum likelihood estimation method was adopted for SEM model fitting. The model fit was assessed using several goodness-of-fit indices, including the CFI (comparative fit index), RMSEA (root mean squared error of approximation), and root mean square residual (SRMR). An SRMR lower than 0.05, an RMSEA lower than 0.08, and a CFI approximating one indicates a good fit. The model will be revised iteratively by deleting or changing nonsignificant ($p > 0.05$) paths during the fitting process. If multiple models pass the criterion, the best goodness-of-fit indices will be selected (Xie et al., 2020; Yang et al., 2021).

iii. 2.3.3 Copula functions

To further reveal the response relationship found in the SEM and to explore how water quality is influenced by water quantity, we applied copula functions to establish a two-dimensional joint distribution of water quantity and quality. The copula function is widely used for constructing multivariate joint probability distributions, which connect the marginal distributions of several random variables. Let F be an n-dimensional distribution function with marginal distributions of each variable denoted as $F_1(x_1)$, $F_2(x_2)$,..., $F_n(x_n)$. Then the joint distribution *F* of *n* random variables X_1, X_2, ..., X_n (where $X_i \in R$ for all i) can be written as Eq. (3):

$$F(x_1, x_2, \ldots, x_n) = P\{X_1 \le x_1, X_2 \le x_2, \ldots, X_n \le x_n\} = C[F_1(x_1), F_2(x_2), \ldots, F_n(x_n)] \quad (3)$$

where X_1, X_2, ..., X_n are observed random variables, and $F_1(x_1)$, $F_2(x_2)$, …, $F_n(x_n)$ is the marginal distribution function of each variable. C is an n-dimensional copula function. This paper used five functions from two common copula families (see Table 1). First, we employed nonparametric methods to approximate the distribution types of the population for determining suitable copula functions (Table S1). The histogram of the water quality-water quantity relationship was used to define the sample population distribution.

Table 1. The full equations of five candidate copulas.

Function type	Copula class	Equation
Gaussian Copula	Meta-elliptical Copula	$C(u,v) = \Phi_2[\Phi^{-1}(u), \Phi^{-1}(v); \rho]$
t-Copula		$C(u,v) = T_2[t_v^{-1}(u), t_v^{-1}(v); \rho]$
Clayton Copula	Archimedean Copula	$C(u,v) = (u^{-\rho} + v^{-\rho} - 1)^{-\frac{1}{\rho}}$

Gumbel Copula $$C(u,v) = \exp[-((-\log(u))^{\theta} + (-\log(v))^{\theta})^{\frac{1}{\theta}}]$$

Frank Copula $$C(u,v) = -\frac{1}{\theta} * \log\left(1 + \frac{(\exp(-\theta u) - 1)(\exp(-\theta * v) - 1)}{\exp(-\theta) - 1}\right)$$

iv. 2.3.4 Generalized additive model

The generalized additive model (GAM) is a nonparametric statistical model exploring the nonlinear relationship between response and explanatory variables (Beale et al., 2010; Pearce et al., 2011). The general formula of GAM can be expressed as follows:

$$G\,(y) = s0 + s1(x1) + \cdots + s^{m}(xm) + \varepsilon \tag{4}$$

s(x) is a smooth function connecting explanatory variables, and ε is a random residual.

The steps for performing GAM analysis are summarized below. First, we analyzed the collinearity of the predictor variables based on the variance inflation factor (VIF; 0<VIF<10 for no multicollinearity; 10 ≤ VIF<100 for strong multicollinearity; VIF ≥ 100 for severe multicollinearity). Second, the potential colinear variables were eliminated according to estimated collinearity, and the connection function was determined according to the type of probability density distribution of the response variable. Third, all remaining variables were included in the GAM model. The degrees of freedom (edf) and significance (p) of the smoothing function were determined, and the determination coefficient (adj-R^2) was adjusted to attain the Akaike's information criterion (AIC) of each driving factor. The insignificant variables were gradually eliminated through the p-value. The smooth functions for predictor variables are based on natural splines. The parameters of the smoothing functions are determined by balancing the Generalized Cross-Validation (GCV) criterion to maximize model explanatory power and prevent overfitting. Finally, the GAM check function was used to evaluate the performance of the optimized model, and the most critical influencing factors were identified according to the edf of the smoothing function of each variable (Chen et al., 2020; Liu et al., 2020).

(iv) 3. Results and Discussion

a) 3.1 Changes in algal blooms in Hulun Lake

This section summarized the results of algal blooms identified from remote sensing and sediment diatoms. Figure 4 illustrates the annual changes of MBE and BO. From 1990 to 2019, both MBE and BO showed periodic fluctuations. Specifically, the algal bloom area varied significantly, with an evident peak in 2000 (Fig. 4). This trend escalated notably from 2001 to 2010, with the maximum area increased by a factor of 16, and the period from 2013 to 2019 had an initial increase followed by a decrease in MBE. From 1990 to 2019, except for 2000, the BO experienced a marked rise, reaching a maximum of 23.6%, with the majority of algal blooms frequency in Hulun Lake being approximately 10%.

The F-statistic and p-values from the structural change test further confirmed the significance of such changes. The mutation points for MBE occurred in 2000, while for BO in approximately 1998 and 2002, which is consistent with Fang et al. (2018), who also found the primary outbreaks in Hulun Lake in 2000 and 2010. Before 2000, due to minor changes in water levels, the variation in the percentage of algal blooms and their area dynamics were consistent, maintaining an inconspicuous trend (Fang et al., 2018). Moreover, according to our previous studies, 1997 was identified as a critical point of change in water levels (Huang et al., 2023), with the period up to 2020 characterized by significant fluctuations. There were two abrupt changes in BO between 1998 and 2002, further confirming the driving force of water level changes. After 2009, the consistency between area changes and the percentage of algal blooms became fragile. MBE's increasing and then decreasing trend indicated that, alongside water level recovery and water quality changes, MBE and BO also underwent synchronous changes.

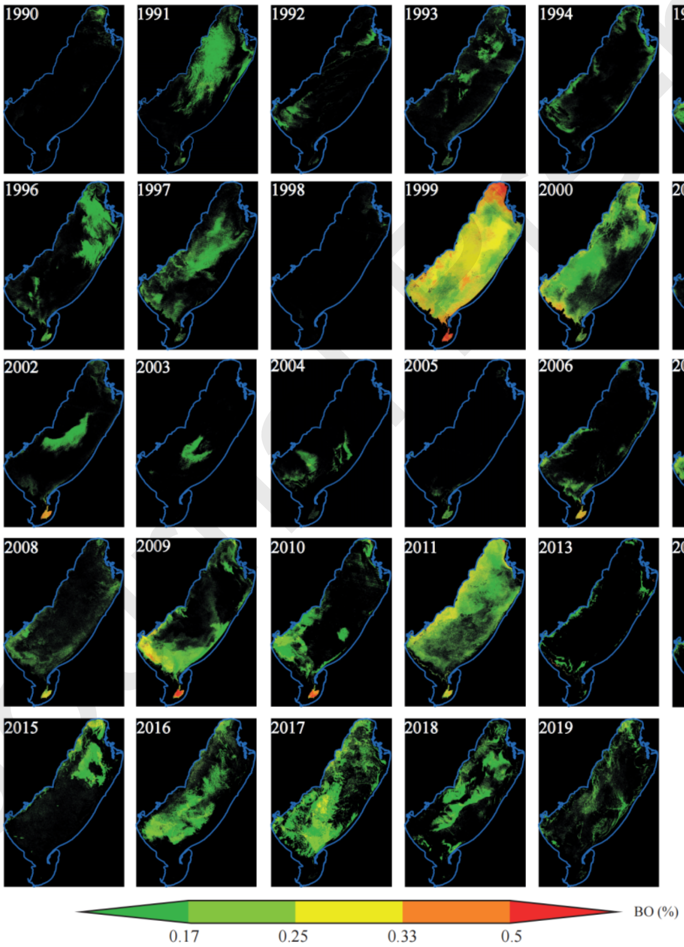

Fig. 4. Spatiotemporal monitoring of algal bloom outbreaks from 1990 to 2019 in Hulun Lake. Black areas indicated regions where algal blooms were not detected or where data was invalid, as reflected by the number of valid images (Nvalid)

Fig. 5 (a) shows the evolution of four indicators derived from sediment records (i.e., richness and density) and remote sensing (i.e., MBE and BO). Results showed that the past three decades have undergone a periodic fluctuation in diatom richness and density. Since 2010, however, diatom richness and density increased steadily, indicating Hulun Lake's aquatic environment recovery. After 2015, the diatom density slightly decreased while richness continued to grow. By comparing the extracted changes, it was found that the changes in lake algal blooms did not coincide with the mutation points of sediment diatoms. Around 2000, BO and MBE experienced increasing and declining transitions, coinciding with a period of recovery in diatom indicators. Around 2010, fluctuations in BO and MBE were observed alongside an overall upward trend in diatom density and richness. This pattern might be linked to changes in eutrophication levels and indicates that the lake's ecological system was evolving toward a more stable state (Wu et al., 2023).

Additionally, the OLS-CUSUM test was applied to our long-term time series data to assess the stability of the lake ecosystem's parameters. Despite the observed fluctuations in the density and richness of diatoms, the OLS-CUSUM values did not exceed the critical confidence level threshold (α = 0.05 dotted line) (Fig. 5 (b)). This result indicates no significant structural changes have occurred, suggesting that the lake's ecosystem has likely not undergone a steady-state transformation over the past three decades. Given that Hulun Lake has not experienced such a transformation, measures to reduce environmental pressures, such as restoring water levels and optimizing water quality parameters, could enable the ecosystem to recover along its original developmental trajectory. The trend variation offered clues about internal states within the lake's ecosystem. The comparison between the two datasets revealed that sediment diatom richness demonstrated better stability than algal blooms from remote sensing. At the same time, the data on algal blooms captured through remote sensing represents just a snapshot in time. To assess the relationship between algal blooms and the density and richness of sediment diatoms, we calculated the coefficient of determination (R^2) between instances of algal blooms and variations in diatom metrics, incorporating varying lag times to account for the effect of delayed algal blooms on sediment diatoms (refer to Table S2 for details). Our analysis revealed a moderate correlation between the richness of diatoms in the lake's sediments and maximum bloom extent (R^2=0.21, $p < 0.05$). A similarly mild correlation was observed between blooms and diatom density, albeit with a one-year delay. These findings underscore that the algal blooms in Hulun Lake exert a moderate influence on the dynamics of richness and density of diatoms. Diatoms are resilient to environmental changes, potentially contributing to their relative stability amidst fluctuations in water quality and quantity (Hao et al., 2021). Compared with algal blooms, the sediment diatom index having fewer mutation points might explain their stable presence in sediment records over time. In contrast, algal blooms captured by remote sensing are more sensitive to immediate environmental changes and exhibit more significant variability in response to nutrient dynamics and water conditions (Shi et al., 2018). For instance, algal blooms detected via remote sensing but absent from sediment diatom records could indicate short-lived bloom events that do not significantly alter the long-term diatom assemblage (Cui et al., 2021). Alternatively, significant changes in diatom compositions not accompanied by corresponding changes in surface algal bloom intensity could reflect shifts in deeper water or benthic conditions, potentially driven by changes in sedimentation rates or bottom-up ecological processes (Liu et al., 2016). Moreover, due to meteorological factors, especially wind speed, cloud cover, and the timing of satellite overpasses, the highly variable algal bloom frequency and sediment diatom richness did not exhibit consistency. Nevertheless, the exchange and cooperative change of diatoms in sediments and algae in water served as the foundation for algal bloom formation. Therefore, it is necessary to observe the algae changes in Hulun Lake from the dual perspective of algae.

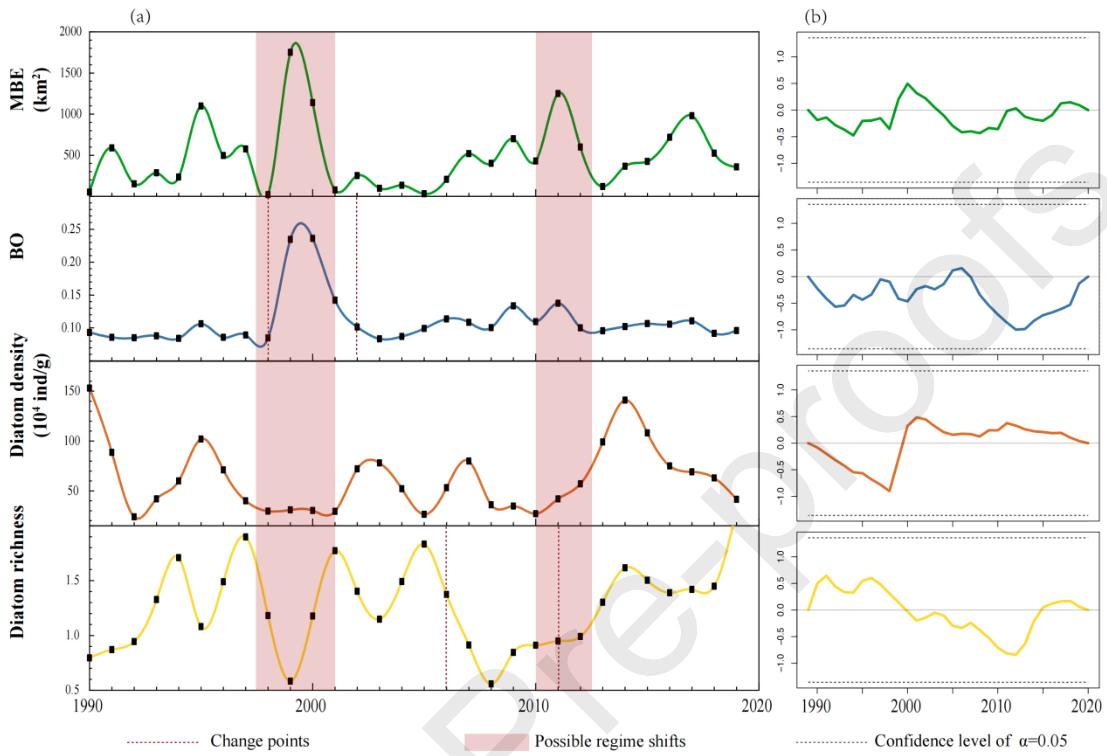

Fig. 5. Change point detection of (a) lake algal blooms and sediment diatom indicators. (b) OLS-CUSUM test on structural changes in diatom composition and diversity.

b) 3.2 The coupling effect of water quantity and quality on algal blooms

In this section, we applied the SEM method to quantitatively explore the driving mechanisms of lake water quality and quantity on both algal bloom phenomena. Figure 6 depicts the derived model, where the thickness of each line is proportional to the standardized path coefficients. Red lines represent positive pathways, while blue ones represent negative ones. Results showed that the selected SEM can explain 92.1% of the variations in diatom density and 87.1% of the variations in diatom richness, with the water quality parameters being the main explanatory factors, namely TP, COD, Chla, and WL. Specifically, WL directly impacted diatom density (effect coefficient: -0.795, $p< 0.001$). TP and Chla had positive effects on diatom density, with standardized path coefficients of 0.757 ($p < 0.001$) and 0.423 ($p < 0.001$), respectively. A similar correlation between diatom density and TP was found by Chen et al. (2021) for Dianchi Lake, while Taihu Lake found a significant negative relationship between TP and diatom density (Shi et al., 2019b). This discrepancy may be attributed to the importance of the nitrogen-to-phosphorus ratio in influencing diatom density (Lai et al., 2011). COD, DO, and LSWT negatively impacted diatom richness, with COD having the most significant effect coefficient of -0.384, while DO and LSWT had effect coefficients of -0.324

and -0.197, respectively. This result suggests that higher concentrations of pollutants are associated with lower diatom richness. Fox et al. (2013) indicate that both excessively high and low levels of COD are detrimental to the stability and integrity of diatom communities. Additionally, studies have shown that WL insignificantly influences diatom richness (Wang et al., 2023). Nevertheless, WL negatively correlated with COD (effect coefficient: -0.607, p = 0.004), and COD negatively influences diatom richness (effect coefficient: -0.384, p < 0.001). This result reflected the impact of the coupled interaction between water quality and quantity on diatom richness. When considering WL as an explanatory variable for changes in diatom density, the identified influence is small (Peng et al., 2021b). Instead, WL indirectly modulates planktonic biomass through interaction with water quality parameters ((Reid and Ogden 2009). The LWST was another crucial factor affecting diatom growth and respiration rates (Kong et al., 2021). Previous studies have indicated that fluctuations in water temperature can influence DO saturation in water, subsequently impacting diatom growth (Da Silva et al., 2005).

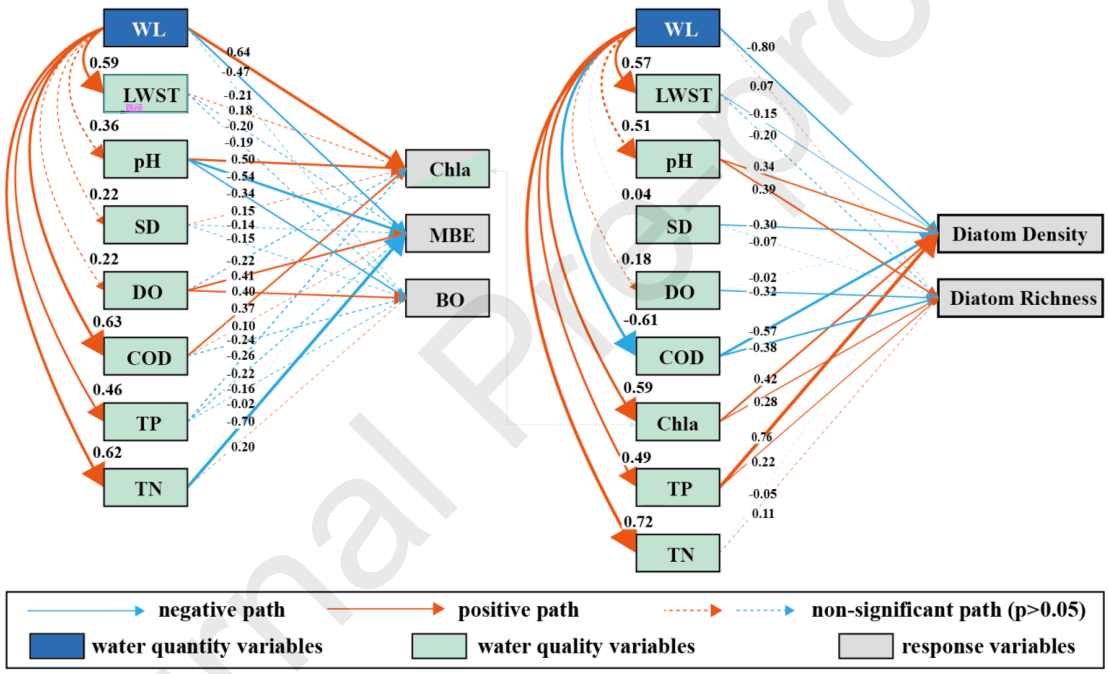

Fig. 6. The structural equation models (SEMs) for Hulun Lake are based on interactions between water quality and quantity, sediment diatoms, and algal bloom variables. Solid lines indicate significant paths, and the thickness is scaled to the strength of the effect; dotted lines represent nonsignificant paths. Red lines show positive path strengths and blue lines show negative path strengths. Overall fit is: chisq=79.76, df=28.00, p< 0.001, CFI=0.620, RMSEA=0.363.

Another SEM was established for MBE, BO, and Chla. The results revealed that coupled water quality and quantity influence could explain 81.7% of the variance in MBE changes. Moreover, the model explained 72.9% of Chla changes and 61.5% of BO changes. Among these, WL emerged as a pivotal influencing factor for both MBE and Chla changes, with standardized path coefficients of -0.47 (p < 0.05) and 0.64 (p < 0.05), respectively. WL is a sensitive predictor of eutrophication and can reflect the lake's capacity to dilute nutrient loads (Liu et al., 2010). In the SEM results, the influence of WL on indicators such as diatom richness and algal bloom frequency was not significant, possibly because WL mostly imposes indirect effects on aquatic ecosystems via its impact on water quality (Wang et al., 2021). A simple instance is the increase in water volume that can facilitate the dilution of nutrients in water, leading to a decrease in algal concentration. Additionally, among the two models, WL has had inconsistent effects on COD in different models. In contrast, in the models with algal bloom and sediment diatoms variables, the relationship was opposite, which showed that although the model structure and path were similar in the established model, However, due to the response relationship between water quality and quantity indexes at different times, the results of different periods may be captured. Similar results have also been found in Poyang Lake and Dongting Lake, and there were positive and negative correlations between water level and COD in the long time series (Geng et al., 2022; Li et al., 2020). These findings underscore the complex interplay between hydrological regulation and nutrient dynamics, ultimately influencing the observed water quality parameters and ecosystem responses. Despite the model's objective to clarify the relative contributions of water quality and quantity to algal bloom dynamics, the fit indices suggest suboptimal model performance. This discrepancy may be attributed to the model not encompassing additional influential variables, such as population and temperature, which have been identified to impact algal blooms (Chen et al., 2021). Integrating these factors notably refines the model's explanatory capability and overall fit.

Notably, TN exhibited a significant positive correlation with MBE among the water quality parameters, with a standardized path coefficient of 0.71 ($p < 0.001$). Negative correlations were observed for pH on both MBE and BO, with standardized path coefficients of -0.54 ($p < 0.001$) and -0.34 ($p < 0.05$), respectively. A similar result was also observed in Taihu Lake, where a strong negative correlation between algal phenology and pH was noted across the entire lake and within specific lake areas (Shi et al., 2019). Chla, however, showed a significant positive correlation (effect coefficient of 0.50, $p < 0.001$). This may be due to the impact of water pH on algal photosynthesis. The weakly alkaline water in Hulun Lake is conducive to algae photosynthesis. Generally, diatom density tends to increase with increasing pH, subsequently increasing the concentration of Chla in water (Kolada, 2014). In addition, the increasing LWST and pH can stimulate algal growth while concurrently limiting sediment diatom growth, ultimately decreasing diatom richness and density (Kong et al., 2021).

c) 3.3 Response analysis between water quality and quantity and identified key response factors

As shown in Fig. 7, joint probability distributions were used to represent the degree of interrelationship and dependence between water level and water quality variables, with dense contours representing high joint probabilities and sparse contours representing low joint probabilities. During periods of low WL, our analysis revealed a low joint probability of observing both low TN concentrations and low WL concurrently (Fig. 7 (a)). This result further supports the possible lack of correlation, implying that the concurrent occurrence of low TN and WL is statistically rare. In particular, at a WL of 543 m, the joint probability density values were higher, indicating that there was a greater likelihood of observing TN concentrations and water levels co-occurring at this specific WL. This may imply a significant relationship or influence between TN concentrations and water levels at this particular WL. As the water level continued to rise (above 544 m), the joint probability gradually decreased, suggesting that the occurrence of specific TN and WL values simultaneously became less likely. Regarding COD variations (Fig. 7 (c)), the probability density curve appeared to be even more tightly distributed than TN. This observation suggested a stronger correlation between these variables within the 542-544 m range. As WL increased, a peak probability density was observed at a water level of 543 m. According to the joint probability distribution of the WL and Chla, when the WL remained constant, the joint probability values increased with increasing Chla concentration. Similarly, when the Chla concentration remained constant, the joint probability values increased with rising water levels. A positive correlation existed between the WL and Chla concentration, implying that as the WL increased, the probability of a higher Chla concentration also increased (Fig. 7 (d)). The primary reason behind this correlation was poorer water quality due to inflow, resulting in outbreaks of algal blooms. Similar situations have been observed in the case of the largest water diversion project globally, the South-North Water Transfer Project (Miyun Reservoir) (Zang et al., 2022). The probability density distribution for the physicochemical indicators of water quality, namely, DO, SD, and pH, exhibited similar trends (Fig. S1).

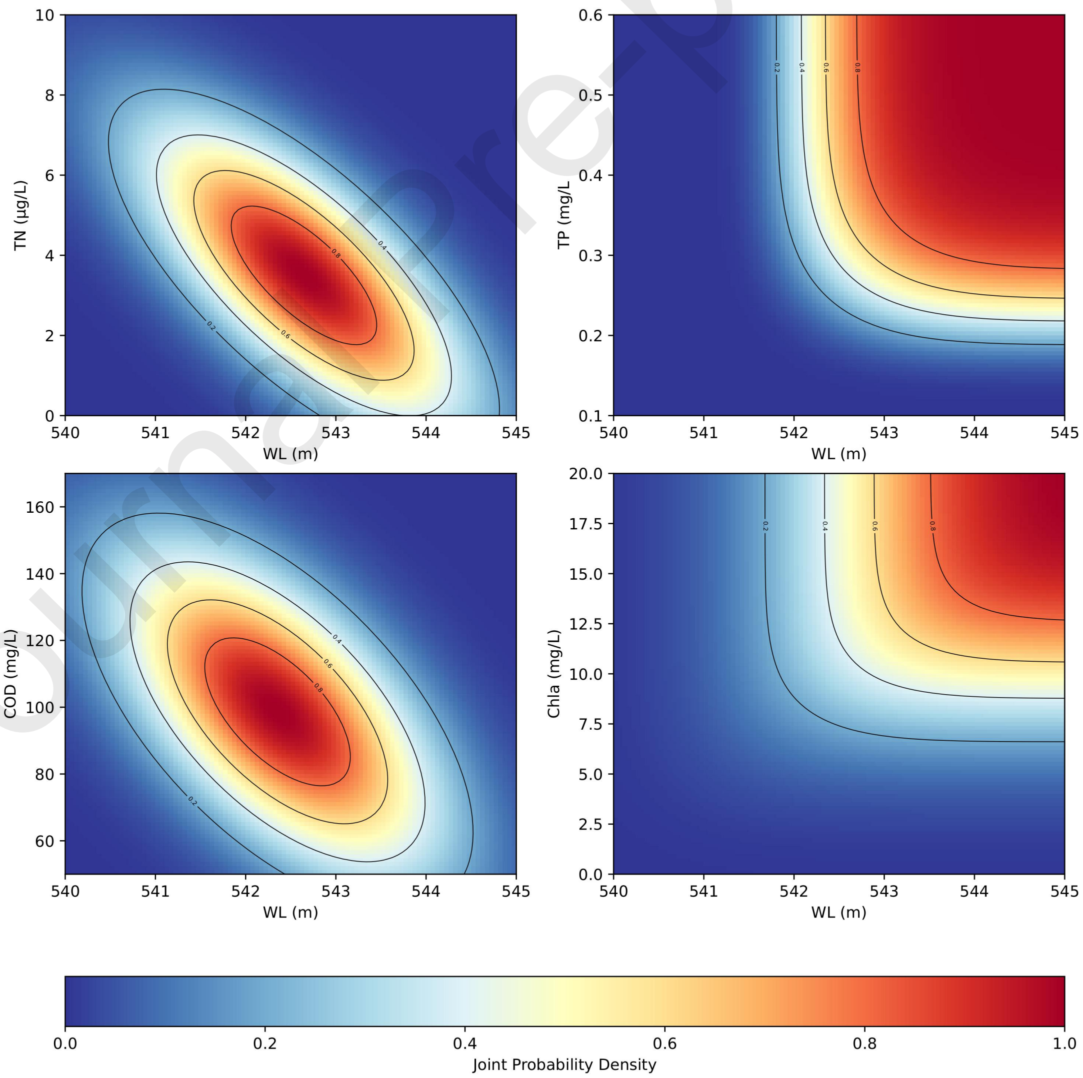

Fig. 7. The best copula probability density distribution function of water quality and water quantity in Hulun Lake.

Next, we applied the GAM model to further explore the nonlinear responses among these factors. According to the fitted results of the GAM (Fig. 8), it was evident that significant nonlinear relationships existed between WL and water quality parameters. The order of explanatory power for other water quality parameters followed TN > COD > Chla (Table 2 and Table S3). The concentration of TN increased with rising water levels. After the WL surpassed 543 m, TN and TP increased with increasing WL. Notably, TN and TP showed more pronounced variations during high-WL periods when WL fluctuated between 543 m and 544 m, marking a high-WL phase. The corresponding change rates for TN and TP were 66.1% and 54.8%, respectively. This could be attributed to reduced runoff and lower water levels, causing the increase in TN to primarily stem from atmospheric deposition and dry deposition into the lake. Meanwhile, the input of TP became less prominent with decreased rainfall and inflow, gradually diminishing the impact of external sources (Yu et al., 2021). Chla increases as the WL increases from 541m to 543 m. However, as the WL further increased beyond 543m, Chla concentration diminished as WL increased. The WL of 543m was a pivotal point where WL and COD transitioned from a negative correlation to a positive one. Within the recovery range of water levels from 541 m to 543m, the dilution effect positively influenced reducing COD (Table S4). SD, DO, and pH responses to WL variations also exhibited insignificant relationships. This indirectly suggested that these three physical indicators could indicate eutrophication effects. Furthermore, the variation in WL, serving as a primary driver of eutrophication, exhibited a less pronounced indirect impact on the changes in SD, DO, and pH within the mentioned range.

Table 2. Parameter results of single-factor meteorological element GAM models for OAC in Hulun Lake

Response variable	Explanatory variables	edf	F	p	dev. expl (%)	Model	R^2
TN	WL	1.87	5.89	0.01	52.5	$g(y) \sim s_{0+}s$ (EVA)+ε	0.46
TP	WL	1.00	2.84	0.11	16.8	$g(y) \sim s_{0+}$ s (AT)+ε	0.11
Chla	WL	2.40	6.39	0.00	39.5	$g(y) \sim s_{0+}$ s (AT)+ε	0.35
COD	WL	1.50	4.73	0.02	44.7	$g(y) \sim s_{0+}$ s (P)+ε	0.39

SD	WL	1.00	0.4	0.538	2.98	$g(y) \sim s_0 + s(Eva) + \varepsilon$	0.05
DO	WL	1.10	0.65	0.409	8.06	$g(y) \sim s_0 + s(AT) + \varepsilon$	0.00
pH	WL	1.81	2.48	0.123	34.3	$g(y) \sim s_0 + s(P) + \varepsilon$	0.25
LWST	WL	1.56	3.83	0.073	29.4	$g(y) \sim s_0 + s(P) + \varepsilon$	0.23

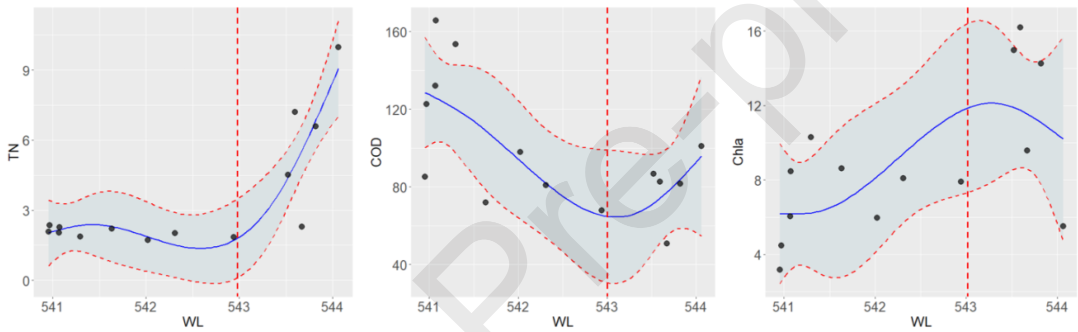

Fig. 8. The fitting function curve of water level variables with response variables based on the GAM model results for water quality in Hulun Lake.

The investigation of pollutant concentrations and fluxes in the Hailaer River, Kherlen River, and Wuerxun River revealed the following long-term trends: the pollutant concentrations from the three inflowing rivers generally displayed an upward trend followed by a subsequent decline from 2011 to 2020 (Fig. 9 (a) and (b)). Upon comparison, it was observed that within the 2011-2020 period, the pollutant flux variations were as follows: the TN and TP levels in the Hailaer River showed a minor upward trend. The TN levels in the Wuerxun River and Kherlen River exhibited a downward trend. In contrast, the TP levels in the Wuerxun River displayed a slight increase, and those in the Kherlen River first experienced a substantial increase followed by stabilized fluctuations. Moreover, it was evident that the water diverted from the Hailaer River contributed over 50% of the total input to Hulun Lake (Fig. 9 (c) and (d)). Since implementing the "river-to-lake" water diversion project, an average annual water replenishment of 750 million cubic meters has been supplied to Hulun Lake through the Hailaer River. Although the river’s water quality had historically been categorized as Class IV (Yue and Wei, 2014), the substantial amount of incoming water presents a significant pollutant source. In post-2013, the inflow from the Hailaer River has markedly contributed to an escalated pollutant loading, leading to a degradation in water quality despite the noticeable increase in water levels. In other words, during the period of water level recovery, pollutant loadings from the diversion project and the natural inflow have played significant roles in the lake's water quality degradation, which deserves further investigation.

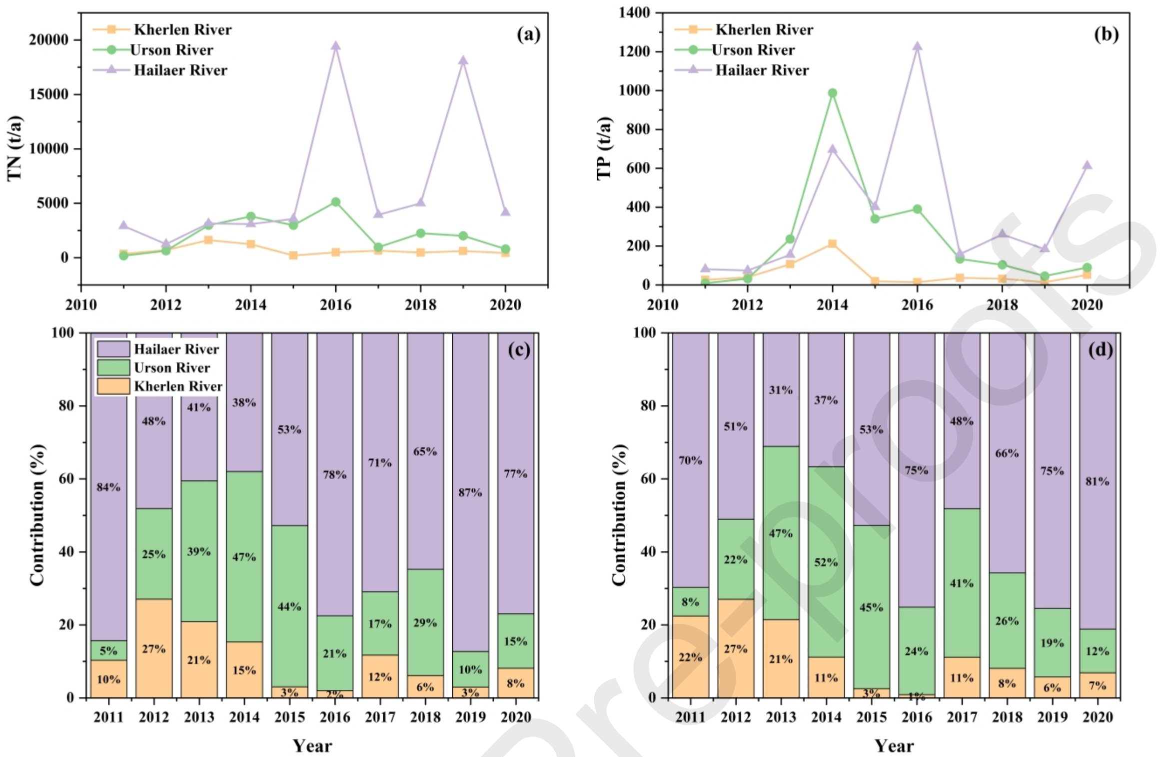

Fig. 9. Annual load and contribution of river pollutants entering Hulun Lake. a) Interannual load change of the river TN in Hulun Lake from 2011 to 2020. b) Interannual TP load changes of rivers entering Hulun Lake from 2011 to 2020. c) TN contribution of rivers entering the lake during 2011-2020. d) TP contribution of rivers entering the lake during 2011-2020.

d) 3.4 Conceptual model for the driving mechanism of algae dynamics

Based on the findings above, a conceptual model was proposed for Hulun Lake to describe the coupling mechanism of water quality and quantity in driving lake algal blooms (Fig. 10). First of all, the results from SEM revealed that the coupling effect of water quality and quantity could explain algal blooms and sediment diatoms. Based on the directional influences of various factors and coupling outcomes, a schematic diagram depicting the long-term mechanism of algal blooms under the coupling of water quality and quantity was constructed (Fig. 10). WL positively affected COD and TN, which in turn positively affected Chla and negatively MBE, respectively. WL exhibited the highest negative influence on diatom density among the algal indicators. Simultaneously, WL affected sediment diatom density and richness through its positive effects on TP and Chla and adverse effects on COD and LWST.

In addition, our Copula functions and GAM models further complement the conceptual model regarding different quality and quantity response periods. Before water diversion, the lake stayed at low water levels, favoring the uplifting process of bottom nutrients to the water surface through mixing. Such a process provided ample nutrients that could accelerate eutrophication and trigger algal blooms. Since the implementation of the water diversion project, water levels have been restored, and nutrient loading has increased since then, which sustained algal growth (Fig. 10). The results from GAM and Copula model showed that when the lake water level reached 543m from the low water level, the Chla concentration continued to rise, the rapid increase in lake nutrient contents and suitable temperatures further enhanced algal growth. From the water level of 543m to the high WL stage, external nutrient loading was reduced, leading to a weakening of algal blooms and eutrophication status, but COD is increasing due to the COD brought by water introduction and driving the covariation in lake algal blooms and sediment diatom assemblages.

Overall, the results from the pivotal role of the 543 m water level in influencing the relationship between water quality and quantity were identified. This relationship exhibited distinct characteristics above and below this threshold. Such differences were especially pronounced during periods of high and low water levels. Additionally, it should be noted that this study focused on water quality and quantity as the most immediate factors influencing algal growth in Hulun Lake, as identified in previous research (Huang, 2023; Zhang, 2022). These studies have acknowledged the significant role of external and climate variables in shaping these factors over the long term. By isolating and directly examining these impacts, we aimed to provide a clearer understanding of how they drive algal dynamics. This approach highlights the specific contributions of internal lake conditions to algal bloom development, offering insights into the underlying mechanisms within the lake. These findings are crucial for informing targeted management practices to control water quality and quantity, addressing algal blooms more effectively.

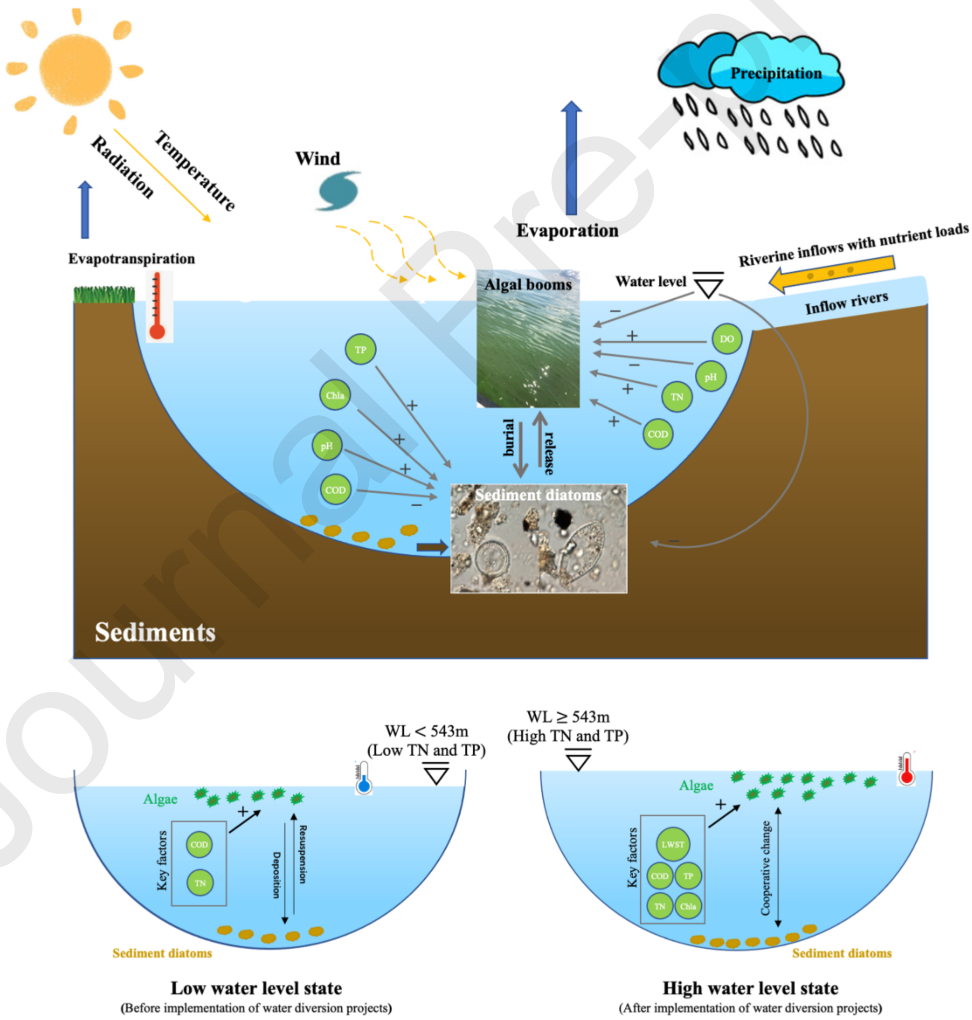

Fig. 10. Influence pathways of water quality and quantity indicators on changes in algal blooms and sediment diatoms and their driving mechanisms.

(v) 4. Conclusions

This study investigated the driving factors behind algal blooms in Hulun Lake by considering both the response relationship and the coupling effects between water quality and quantity. Compared to previous research, our study explored the variability of lake algal blooms at different scales using sediment diatoms and remote images. This approach not only provides a holistic view of the dynamics of lake algal blooms but also leverages the strengths of each method to offer a more comprehensive analysis. Utilizing sediment diatoms and remote sensing images, we identified distinct mutation points in algal bloom dynamics—around 2000 from remote sensing and approximately 2010 from sediment diatoms. Using two datasets, we further explored the coupling effect of water quality and quantity using SEM; 61.5% to 92.1% of the variability in algal blooms could be explained. Among the possible explaining factors, the WL had the highest explanatory power on algal blooms. TP and Chla are secondary factors that positively correlate with algal blooms, while COD and LWST negatively correlate with diatom density and richness. The MBE and BO were positively influenced by TN, COD, and DO while negatively affected by pH. Overall, the coupling effect of water quality and quantity is modulated mainly by WL change. Using copula functions to assess joint probabilities and GAM to delineate nonlinear relationships revealed that a critical water level threshold at 543m significantly influences nutrient dynamics. Above 543m, TN and COD showed upward trends, while Chla displayed a downward trend. However, as the WL recovered beyond 543 m, increased nutrient loads led to rising TN and COD concentrations. This pattern was primarily attributed to longer circulation cycles during low water periods, facilitating the accumulation of nitrogen and phosphorus pollutants. During high water periods, increased nutrient input through water diversion stimulated the growth of phytoplankton in the lake. Therefore, it is essential to regulate water levels appropriately and control key water quality indicators such as TN, TP, and COD to mitigate the risks of eutrophication and algal blooms associated with water level decline. Particular attention is required to understand the changes in water quality during periods of high and low WL.

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Conflicts of Interest:

The authors declare that there are no financial or personal conflicts of interest in this study.

a) Highlights

Dual-scale view of algal blooms: remote sensing image and sediment core sample.

Utilization of multiple analysis methods, including Copula, GAM, and SEM analysis.

The nonlinear water quality and quantity variation exhibited a turning point in water level changes at 543 meters.

Through indirect coupling effects, water level changes dominate water quality shifts, algal blooms, and diatom community variations.