

Spatiotemporal variations of water quality and driver forces detection in Yangtze River Basin, China from 2008 to 2020 by multi-statistical analyses

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Abstract

Water quality deterioration is a prominent issue threatening water security throughout the world. Yangtze River Basin, as the largest river in China, is facing severe water pollution due to the intensive human activities. The analysis of water quality trends and identification of driver factors are significant for sustainable water quality management. Thus, spatiotemporal characteristics of the water quality from 2008 to 2020 were analyzed by using Mann–Kendall test and Rescaled Range analysis (R/S), respectively. Also, the drivers of the key monitoring indicators including permanganate index (COD_{Mn}), ammonia nitrogen ($\text{NH}_3\text{-N}$) and total phosphorus (TP) were detected by multi-statistical analyses. The results showed that water quality was significantly improved, which was reflected from its mean concentration of $\text{NH}_3\text{-N}$ and TP, decreasing from 0.31 mg/L to 0.16 mg/L and 0.16 mg/L to 0.07 mg/L, respectively. However, the concentration of COD_{Mn} did not remarkably decline in the past 13 years. The R/S analysis indicated that the concentration of $\text{NH}_3\text{-N}$ would continue to decrease in the next 13 years, while COD_{Mn} might continue to increase, which should be of great concern to us. In terms of spatial distribution, the water quality in the upstream was significantly better than that of the mid-downstream. Multi-statistical analyses revealed that the temporal evolution of water quality was predominantly influenced by tertiary industry (TI), nitrogen fertilizer application rate (N-FAR), phosphate fertilizer application rate (P-FAR) and irrigation area of arable land (IAAL), with a contribution rate of 15.92%, 14.65%, 3.46% and 2.84% respectively. The spatial distinction of COD_{Mn} was mainly influenced by TI, while TP is primarily determined by anthropogenic activity factors including N-FAR, P-FAR and so on. This study was expected to provide deep insights into water quality evolution and foundations for water quality management in Yangtze River Basin.

1 Introduction

Recently, water pollution is of great concern in global scale (Sun et al. 2019). Since the rapid economic development over the past decades, China's river has suffered water quality impairments due to intensified human activities (Jiacong et al. 2021). Yangtze River Basin is the largest river basin in China and Asia (Yuanchen et al. 2019) and play a significant role in ecological integrity and ecosystem service due to its abundant resources, numerous population agglomeration and fast-growing industrial development (Di et al. 2019). However, Yangtze River Basin is faced with the challenge of maintaining (or improving) water quality while allowing for the economic growth and population expansion (Qin et al. 2014) and the water environment in recent years has improved but still severe. Phosphorus pollution threatens water quality prominently, and the net Anthropogenic Phosphorus Inputs (NAPI) for Yangtze River Basin ($1783 \text{ kg P km}^{-2} \text{ yr}^{-1}$ in 1985-2015) was significantly higher than the average NAPI reported for mainland China ($465 \text{ kg P km}^{-2} \text{ yr}^{-1}$ in 2009) (Hu et al. 2020). Contamination in the mid-down streams has become a serious environmental problem in Yangtze River Basin (Deng et al. 2017, Weili et al. 2018, Zeng & Wu 2013). Also, the river ecosystem is facing biodiversity reduction (Tingui et al. 2020) and decrease in wetlands induced by the lake reclamation, land degradation, and large-scale agricultural development (Sun et al. 2017). Environmental issues in the Yangtze River Basin are highly valued by the

government, thus numerous politics and measures have been enacted to facilitate the economic development and environmental protection. For example, “Outline of the Development Plan for the Yangtze River Economic Belt” was issued in 2016, which emphasized the positive urbanization promotion under environmental capacity (Mao et al. 2021). Furthermore, “Yangtze River Protection Law of the People's Republic of China” that officially implemented on March 1, 2021 stipulated to carry out protection work in the perspective of the entire catchment. Hence, knowledge of water quality evolution and the variation driver mechanisms in Yangtze River Basin are essential to obtain a better understanding of water management measures effectiveness.

Detailed and periodic water monitoring information and related analysis are of great significance for assessment of water quality (Xiong et al. 2020). The spatiotemporal variation pattern of the monitoring data in different river ecosystems was generally clarified by Mann–Kendall test (Ma et al. 2020, Weili et al. 2018, Zhai et al. 2014), time-series decomposition (Weili et al. 2018), Water Quality Index (WQI) (Jiacong et al. 2021, Wu et al. 2018) and Moran Index (Zhai et al. 2014), etc. These studies revealed that water quality has been improved remarkably in China due to the reduced discharges from both industrial, rural, and urban residential sectors, but not the increasing agricultural discharge (Ma et al. 2020). In terms of the spatial differences, rivers in eastern China showed relatively poorer water quality, TP and NH₃-N contributed over 85% for the impaired condition, respectively (Jiacong et al. 2021). More detailed, the water quality was considered as “moderate” (WQI values 50-70) in Taihu basin from 2014 to 2016 (Wu et al. 2018). In Yangtze River Basin, it showed gradual improvement in water quality during 2004-2015 and greater improvement in the uppermost basin (Weili et al. 2018). Overall, water quality analyses in the river ecosystem mainly focused on the main indicators of COD_{Mn}, NH₃-N and TP (Di et al. 2019, Hu et al. 2020), and it was always concentrated on mainstream or specific monitoring sections of Yangtze River Basin ecosystem (Weili et al. 2018, Wu et al. 2021b, Wu et al. 2018). That is to say, the comprehensive understanding for the entire basin during a long time series are poorly studied. Moreover, there is a more urgent need for the driving mechanism behind the spatiotemporal variation trend in order to give deep insight into the water quality evolution and provide more information for the water environment management.

The dynamics of inland water quality might be determined by anthropogenic activity factors such as waste water discharge (Weili et al. 2018), point source pollution (Zhai et al. 2014), water treatment capacity (Jiacong et al. 2021), fertilizer application (Zhou et al. 2021) and so on. It was also proved that the nitrogen cycle was associated with the hydrological regime at the basin level (Yi et al. 2017). What's more, rapid economic development might have an impact on water quality (Weili et al. 2018). Thus, it is inferred that economic factors (GDP, primary industry, secondary industry, tertiary industry, population density, etc.) could be included in the drivers range (Zhou et al. 2021). It was also confirmed the operation of the Three Gorges Dam affected the water discharge in Yangtze River Basin (Guo et al. 2011) and thus it is indispensable to explore the inner relationship between water quality and the reservoirs. In terms of analysis methods, the multi-statistical analyses including Spearman (Sun et al. 2019) or Pearson (Zhou et al. 2021) correlation analysis, multiple linear regression (Li et al. 2020, Ma et al. 2020, Zhai et al. 2014)

and principal component analysis (PCA) (Ma et al. 2020, Sun et al. 2019) were commonly used to detect the driver factors of the water quality evolution. Furthermore, most studies focused on qualitative analysis, quantitative analyses of contributions of driver factors to the dynamics of water quality were scarcely studied.

In order to study the variation trend of water environmental quality and evaluate the effectiveness of previous governance, our study comprehensively evaluated water quality in spatial-temporal dimension in the whole catchment from 2008 to 2020 and further explored their driver factors. The drivers in our study included meteorological, anthropogenic activity, land use and socioeconomic factors based on the information mentioned above and listed in detail in section 2.4. Furthermore, multi-analysis methods such as correlation analysis, Redundancy analysis (RDA analysis) and multiple linear regression (more detailed in section 2.5) were applied to detect the key drivers of these spatial-temporal changes. This study could provide deep insights into water quality evolution and the main driving factors behind it, which could further provide references for the water quality management of Yangtze River.

2 Materials And Methods

2.1 Study area

Yangtze river, with the estimated length of 6300 km, originates from Tanggula Mountain in Qinghai Province, and merges into the East China Sea. Its total catchment area is 1.8 million km², accounting for 18.8% of the total land area in China (Tian et al. 2019). Yangtze river flows through 19 provinces and thus shows high natural characteristics complexity. In order to monitor the dynamic of the water quality of Yangtze River, the government started to build automatic monitoring stations since 1984, which has been developed into a total number of 1007 by July, 2020 and covers a large area from the upper to lower reaches (Figure S1).

2.2 Water quality data source

Water quality monitoring data from the automatic monitoring stations (Figure S1) in the Yangtze River Basin was obtained from the National Surface Water Environmental Quality Monitoring Network (<http://www.cnemc.cn/sss/szzdjcssj/>). The large dataset measured every four hours from January 2008 to July 2020 was used to collect the water quality variation. The information in each monitoring station included site code, site name, monitoring time and the monitoring value. The monitoring values include basic physicochemical parameters of pH, water temperature, turbidity, conductivity, and water quality parameters of dissolved oxygen (DO), ammonia nitrogen (NH₃-N), total nitrogen (TN), total phosphorus (TP), permanganate index (COD_{Mn}).

2.3 Trend analysis and prediction for water quality data

Water quality data was preprocessed including data complement, abnormal values and null values handle into the form of daily, monthly, and annual average by R-studio. In order to determine the change

trend of water quality in the recent years and predict their changes in the future, the Mann-Kendall (M-K) test and the Rescaled Range (R/S) analysis were conducted for the main monitoring indicators including COD_{Mn} and NH_3-N (There were limitations in the analysis of TP due to the missing value) (Table 1), respectively. The water quality was evaluated by worst factor water quality assessment method according to "Surface Water Environmental Quality Standard" (GB3838-2002) and then the spatial heterogeneity of the main monitoring indicators (COD_{Mn} , NH_3-N , TP) was studied by ArcGIS.

Annual water quality data was processed by M-K test and its mutation test to reveal their variation trend. In M-K test, the main equations are listed as follows:

$$S = \sum_{k=1}^{n-1} \sum_{j=k+1}^n \text{sgn}(x_j - x_k) \quad (1)$$

$$\text{sgn}(x_j - x_k) = \begin{cases} 1, & (x_j - x_k) > 0 \\ 0, & (x_j - x_k) = 0 \\ -1, & (x_j - x_k) < 0 \end{cases} \quad (2)$$

$$Z = \begin{cases} \frac{s-1}{\sqrt{VAR}} S > 0 \\ 0 S = 0 \\ \frac{s+1}{\sqrt{VAR}} S < 0 \end{cases} \quad (3)$$

For the time series (x_1, x_2, \dots, x_n) , S is the test statistic and reflects normal distribution. VAR is the variance which is equal to $n(n-1)(2n+5)/18$. n is the sample number. There is the suppose H_0 that the time series are independent and equally distributed. Under a given confidence level α , if $|Z| \geq Z_{1-\alpha/2}$, H_0 is not accepted and the data shows an obvious change trend. $Z > 0$ indicates an upward trend, while $Z < 0$ reflects a downward trend (Hirsch et al. 1982).

Table 1
The annual average data of COD_{Mn}, NH₃-N and DO from
2008 to 2020 in Yangtze River

Year	NH ₃ -N (mg/L)	COD _{Mn} (mg/L)	DO (mg/L)
2008	0.28±0.25	2.22±0.87	7.90±1.79
2009	0.29±0.49	2.27±1.47	8.00±1.68
2010	0.28±0.48	2.25±0.90	8.00±1.62
2011	0.31±0.32	2.15±0.88	8.02±1.80
2012	0.26±0.23	2.11±0.91	8.26±1.70
2013	0.24±0.31	2.26±1.21	8.13±1.70
2014	0.24±0.21	2.14±0.98	8.19±1.77
2015	0.25±0.24	2.29±0.94	8.61±1.83
2016	0.31±0.30	2.53±1.48	8.15±1.86
2017	0.30±0.58	2.63±2.18	8.05±2.27
2018	0.24±0.50	2.65±2.02	8.41±2.11
2019	0.20±0.73	2.75±3.40	8.09±2.16
2020	0.16±0.30	2.51±1.64	8.50±2.21

Then, the mutation point was further carried out by using of M-K mutation test. UF_K and UB_K were calculated by processing the time series in the positive and reverse order. $UF_K > 0$ indicates an upward trend, while $UF_K < 0$ demonstrates a downward trend. It indicates a distinct upward or downward trend when the UF_K exceeds the critical value line ($U_{0.05} = \pm 1.96$). Mutation point occurs when UF_K and UB_K intersects.

Variation trend of the time series $\xi(t)$ ($t = 1, 2, 3, 4, \dots$) in the future was predicted by R/S analysis.

$$\langle \xi \rangle_n = \frac{1}{n} \sum_{t=1}^n \xi(t) \quad (4)$$

$$X(t, n) = \sum_{\mu=1}^t (\xi(\mu) - \langle \xi \rangle_n) \quad 1 \leq t \leq n \quad (5)$$

$$R(n) = \max_{1 \leq t \leq n} X(t, n) - \min_{1 \leq t \leq n} X(t, n) \quad (6)$$

$$S(n) = \sqrt{\frac{\sum_{t=1}^n (\xi(t) - \langle \xi \rangle_n)^2}{n}} \quad (7)$$

$$R/S = cn^H \quad (8)$$

In the equations 4-8, $\langle \xi \rangle_n$ is the mean series of $\xi(t)$, $X(t, n)$ is cumulative deviation series. R is the range of $X(t, n)$. S is the standard deviation of $\xi(t)$. It is proved that R/S has a relationship as equation 8 by Hurst(Xu et al. 2004). H is the Hurst index which reflects whether the variation processes have “memorable”. There shows no correlation between changes of the past and future while H=0.5. If H>0.5, The time series presents a positive continuity, that is, the future variation trend is identical to the current. while H<0.5, it shows the opposite.

2.4 Anthropogenic discharge data and impact variables

The Yangtze River Basin, with the estimated length of 6300 km, spans 19 provinces, municipalities, and autonomous regions across eastern, central, and western China (Chen et al. 2020). However, the partial affiliation (not all) of each province with the Yangtze River Basin brings certain challenges to the collection of driving factors. To improve the accuracy of the analysis, the data was acquired from the "China Meteorological Yearbook" and "Yangtze River Yearbook" from 2008 to 2020 based on parts of each province belonging to Yangtze River Basin rather than the whole province. In this study, the drivers were divided into meteorological, anthropogenic activity, land use and socioeconomic factors. Meteorological factor included precipitation (Pre) and water temperature (WT). Anthropogenic activity information was consisted of total wastewater discharge (TWD), investment in water conservancy, environment and public facilities management industry (I in WEPM), total water resources (TWR), nitrogen and phosphate fertilizer application rate (N-FAR and P-FAR respectively) and reservoirs numbers (R). Land use factors included wetland area (WA) and irrigation area of arable land (IAAL). Socioeconomic data was composed of primary industry (PI), secondary industry (SI), tertiary industry (TI) and population (Table S1).

2.5 Statistical analysis for the driving factors of water quality dynamics

Multi-statistical analyses such as Pearson correlation analysis, multiple linear regression and RDA analysis were used to demonstrate the driving factors of COD_{Mn} , $\text{NH}_3\text{-N}$ and TP in spatiotemporal variation. Pearson index was calculated to initially determine the correlation between monitoring indicators and the driving factors in a qualitative perspective (Li et al. 2019). Multiple linear regression was conducted to identify drivers of spatial heterogeneity.

RDA analysis was further used to quantify the correlation between indicators of COD_{Mn} , $\text{NH}_3\text{-N}$ and TP and driving factors (Naveedullah et al. 2016). Forward factor selection was operated after testing significance by each factor and calculating variance expansion coefficient to mitigate the effects of collinearity. Furthermore, Hierarchical segmentation was used to obtain the R^2 (conditional effect)

assigned to each explanatory variable to determine the main drivers. Statistical analysis was all conducted in R-studio.

3 Results And Discussion

3.1 Temporal dynamics of water quality parameters from 2008 to 2020

The concentration of COD_{Mn} and $\text{NH}_3\text{-N}$ from 2008-2020 in Yangtze River generally showed an increasing and decreasing trend, respectively from the result of M-K test, which showed the Z value of 2.50 and -2.01, under the premise of passing the 95% confidence test. In addition, the mutation test showed that $\text{NH}_3\text{-N}$ increased from 2008 to 2012 and decreased from 2012 to 2020 (especially from 2017), with the mutation points appeared in 2013 and 2015. This was possibly owing to the strict control of $\text{NH}_3\text{-N}$ since the government conducted a three-level zoning system (basin-control area-control unit) and treated $\text{NH}_3\text{-N}$ as a binding indicator for total control during 12th five-year plan (Zhang et al. 2019). In contrast, the concentration of COD_{Mn} showed an increasing trend from 2008 to 2010, and a decreasing trend in the next 5 years. What is strikingly noticeable is its increasing trend from 2016 and even exceeded the upper critical limit ($\alpha = 0.05$, indicating an obvious variation trend) in 2018 (Figure 1). It was reported that the impact of human activities has been intensified and the discharge of organic pollutants has become increasingly prominent in Yangtze River Basin (Zhu et al. 2020), which could cause the increasing trend of the COD_{Mn} . Another possible explanation was that a regional flood occurred in Yangtze River Basin caused by El Niño event (Cao et al. 2017, Xiao et al. 2015) in 2016, which might cause a sudden addition for COD_{Mn} in rivers through a large quantity of reducing substances washing into the waterbody (Zhang & Zhi 2020). Bai, et al. has also proved that the living sources and non-point agricultural sources have greater COD_{Mn} contribution rates in the wet season (Bai et al. 2021). Thus, the increase of COD_{Mn} in Yangtze River Basin might be caused by both human discharge and precipitation, which would be further explored in section 3.3.

We further explored the possible dynamic trends in the future by using of R/S analysis. The results revealed a positive sequence of COD_{Mn} and $\text{NH}_3\text{-N}$ in time series, which could be observed through the H value (0.9078 for COD_{Mn} and 0.7902 for $\text{NH}_3\text{-N}$, both greater than 0.5) (Figure S2). Combined with the result of M-K test, the concentration of $\text{NH}_3\text{-N}$ would continue to decrease, while COD_{Mn} might statistically continue to show significant increase. Despite the slight improvement of the water quality of the Yangtze River, COD_{Mn} still showed an increasing trend in the future, which might induce eutrophication issues due to the rising organic loads (Li et al. 2021b). That is to say, COD_{Mn} pollution could further deteriorate in the next 13 years if no effective measures were implemented. Hence, it deserves our great attention to reduce the discharge of oxygen-consuming pollutants into rivers and decrease the concentration of COD_{Mn} in Yangtze River in the future.

In order to get more knowledge of the temporal dynamics of water quality, the seasonal trend of major parameters was also investigated. The concentration of TN and COD_{Mn} showed remarkable seasonal change trend. Specifically speaking, COD_{Mn} showed an increasing trend from January to July and downward trend from August to December, while TN showed an opposite trend (Figure 2). It has been proposed that point source pollution concentration shows the characteristic of dry season > normal season > wet season in turn, while non-point source pollution presents the opposite (Bai et al. 2021). In Yangtze River Basin, the multi-terraced terrain resulted in complicated climate status, against a general background of dry winter and wet summer (Li et al. 2021c). In terms of this background, COD_{Mn} and TP maintain a high concentration level in summer induced by the scouring of the reducing substances and phosphorus-containing compounds into water environment, while NH₃-N declined owing to the dilution of the rain. This view was also consistent with that of Wu, et al (Wu et al. 2021a). Thus, it could be preliminary concluded that COD_{Mn} and TP might mainly originate from non-point source such as agricultural source (Bai et al. 2021) et cetera, while NH₃-N was from point source. Additionally, the detailed correlation between COD_{Mn} and precipitation would be further discussed in Section 3.3.

Previous study proposed that the increased input of the dominant sources of TP including agriculture, wastewater, or stormwater into lakes and streams might contribute to the observed increased TP (Stoddard et al. 2016). Phosphorus and suspended sediment (SS) are closely related in the water body (Dong et al. 2020). Compared with the dissolved state, the particulate phosphorus is easier to be adsorbed by SS. Thus, the high concentration of TP in moist season might also be attributed that the main form of TP was particulate phosphorus in Yangtze River Basin. Additionally, there were also statements that the higher organic matters concentration in summer might be induced by the biological activities in high temperature (Li et al. 2021b).

What's more, NH₃-N and COD_{Mn} did not display poor water quality worse than Class II, but TP exceeded the standard of Class III (Figure 2). Therefore, the excessive total phosphorus is still a prominent environmental problem in Yangtze River Basin, which should be paid more attention.

Based on the major monitoring water parameters (DO, COD_{Mn}, TP and NH₃-N), the water quality in recent years was assessed according to worst factor water quality assessment method. The proportion of the auto-monitoring sites whose water quality better than class Ⅴ standard increased from 85–96% from 2016 to 2020 (Figure S3). Those sites worse than Class V standard decreased significantly from 5% to 0, and even eliminated in 2020. Overall, the results revealed that water quality impairment has relieved during the previous period. However, still several parameters exceeding the class Ⅴ standard. TP and COD_{Mn} were the main over-standard factor from 2016 to 2020, with exceedance rate (worse than class Ⅴ) 2.4% (with a total number of exceeding sites of 53 in 2219) and 2.1% (with a total number of exceeding sites of 47 in 2219) respectively. Despite their over-standard state, the mean concentration of NH₃-N and TP has actually decreased from 0.31mg/L to 0.16mg/L and 0.16mg/L to 0.07mg/L, respectively. Thus, the water quality has improved significantly in terms of the decrease of the proportion of the sites worse than class V and the main over-standard factor concentration, which revealed that numerous water

quality strategies in Yangtze River Basin come into effect. It was reported that enormous effort such as an ever-improving legal system and the popularity of sewage treatment plants and so on leads to improving water quality (Weili et al. 2018), which was also reflected in the water quality improvement in Yangtze River Basin.

3.2 Spatial heterogeneity of water quality parameters in Yangtze River Basin

Large area coverage across 19 provinces in Yangtze River Basin leads to the spatial heterogeneity of the water quality. Thus, it is necessary to explore the spatial distinction of individual sites. The results indicated that the number of the sample sites exceeding the standard class III for COD_{Mn} accounted for 4% (22 in 551) in all the studied sites. The average concentration of COD_{Mn} in exceeded sites was 7.15 mg/L, with an exceeding factor of 0.19. COD_{Mn} in the middle (2.62 mg/L) and lower reaches (3.29 mg/L) displayed higher concentration than that in the upper reaches (2.14 mg/L), although the concentration of COD_{Mn} in the all sites were better than Class III (Figure 3). Higher COD_{Mn} monitoring concentrations were observed in Hubei, Jiangsu and Chongqing, especially in Hubei province, whose ratio was nearly 50% in the 3 provinces. Hubei province was located in the border of middle (more proportion) and upper reaches with large distribution of rivers and lakes. As a large amount of upstream water entered, the river course became narrow and the flow rate slowed down, which affected the self-purification capacity and its water quality further. The average value of $\text{NH}_3\text{-N}$ was 0.15 mg/L in the upstream and 0.29 mg/L in the mid-downstream, respectively. The number of exceeded sites occupied 1% (5 in 524) in all sampling sites, with an exceeding factor of 0.41. It could be found the spatial variation of $\text{NH}_3\text{-N}$ and COD_{Mn} were similar, which all revealed that they may come from the same source such as industrial and domestic emissions (Xia et al. 2018). In addition, Bai et al. studied that the main pollutant sources of COD and $\text{NH}_3\text{-N}$ in 2019 in the Tuojiang River Basin were rural living point sources and urban living point sources (Bai et al. 2021). Wang et al. also pointed out that urbanization and population density could affect the level of pollution (Wang et al. 2007). Thus, rapid economic development and high population density in Hubei and Jiangsu province might lead to higher discharge of domestic and industrial sewage, which might cause their higher concentration of $\text{NH}_3\text{-N}$ and COD_{Mn} than other provinces. Furthermore, due to the fast-growing economy and formidable population aggregation ability in Yangtze River Delta (Xu et al. 2018), the concentration of COD_{Mn} and $\text{NH}_3\text{-N}$ were higher in the mid-downstream compared with the upstream. On the other hand, this spatial heterogeneity could also be explained by the reason that the upstream water might have a strong purification capacity which depends on biological activity, water residence time and the area of mineral surfaces exposed to water (Semenov et al. 2019), and can be restored as soon as possible without external pollution.

Phosphorus, as the important indicator in the water quality management, is the first controlling element that restricts algae growth in most fresh water, and thus an important factor that causes water eutrophication (Dong et al. 2020). In the spatial scale, TP was evaluated by lake and reservoir standards since the slow flow in Yangtze River Basin induced by diversion, transfer, and connection between rivers

and lakes. Under this standard, there would be 57.2% (315 in 551) monitoring sites that exceed the class III standard limit (0.05 mg/L), which should be concerned. It was reported the use of large-scale chemical fertilizer in Yangtze River Basin would cause the increase concentration of the dissolved inorganic phosphate (DIP) (Dai et al. 2011). Additionally, phosphate rock, fertilizer and plaster enterprises mostly distributed in the upper and middle reaches, which could lead to the discharge of pollutants during the production process. Thus, TP showed higher concentration in upstream (0.17 mg/L) than that in mid-downstream (0.11 mg/L). According to the statistics, the reserves of phosphate rock and fertilizer enterprises in Hubei, Hunan, Yunnan, Guizhou and Sichuan provinces accounted for 99.1% and 95.5% respectively in 2019. TP in these provinces presented high level concentration relevantly. It has been found China is the world's largest supplier of P-containing rock, and mining-induced P changes are seen in many lakes of Western China (Tong et al. 2017). What's more, there are numerous of studies proved that the agricultural sources are the main sources for TP (Bai et al. 2021, Di et al. 2019). Hence, in the process of mining and fertilizer production, sewage and wastewater discharge would increase the concentration of TP and affect the water environment. Combined with the speculation of the TP pollution source in section 3.1, TP pollution should be paid more attention and measures to control non-point source pollution should be taken to further control it.

3.3 Main driver detection for temporal dynamics in Yangtze River from 2008 to 2020

In order to determine the relationship from a qualitative perspective, Pearson correlation analysis was conducted between the drivers and the water quality data (COD_{Mn} , $\text{NH}_3\text{-N}$, TP). The results showed that COD_{Mn} and $\text{NH}_3\text{-N}$ had a synergistic variation ($r=0.3827$, $p<0.05$) (Figure 4), which indicated that oxygen-consuming organics COD_{Mn} and $\text{NH}_3\text{-N}$ might come from same pollution source, consistent with the studies of Bai et al (Bai et al. 2021). COD_{Mn} and TP was negatively correlated ($r=-0.2748$, $p<0.05$), thus, the treatment of a certain pollutants should also consider the impacts from other pollutants.

DO was negatively related with COD_{Mn} ($r=-0.3101$, $p<0.05$), $\text{NH}_3\text{-N}$ ($r=-0.3451$, $p<0.05$) and TP ($r=-0.3167$, $p<0.05$), respectively, indicating that an oxygen-deficient state occurred induced by the large oxygen consumption in the waters with higher concentration of COD_{Mn} , $\text{NH}_3\text{-N}$ and TP. Generally, the black-odorous water was formed due to the dissolved oxygen deficiency (Liang et al. 2018), which was common observed in the southern China. Thus, control of the COD_{Mn} and $\text{NH}_3\text{-N}$ could help the management of the urban black-odorous waters.

As for the correlation between water quality data and the drivers, both COD_{Mn} and $\text{NH}_3\text{-N}$ showed negative correlation with pH ($r=-0.1913$, $p<0.05$ for COD_{Mn} and $r=-0.3540$, $p<0.05$ for $\text{NH}_3\text{-N}$), N-FAR ($r=-0.2371$, $p<0.05$ for COD_{Mn} and $r=-0.3979$, $p<0.05$ for $\text{NH}_3\text{-N}$) and P-FAR ($r=-0.2137$, $p<0.05$ for COD_{Mn} and $r=-0.3788$, $p<0.05$ for $\text{NH}_3\text{-N}$). The three drivers displayed higher correlation coefficient with $\text{NH}_3\text{-N}$ compared with COD_{Mn} and they were also inferred to be the main drivers of the COD_{Mn} and $\text{NH}_3\text{-N}$ temporal variation. COD_{Mn} positively related to TI ($r=0.4263$, $p<0.05$) and SI ($r=0.2624$, $p<0.05$), which

revealed that the rapid development of secondary and tertiary industry might lead to increased intensity pollution of COD_{Mn} . This was consistent with the results revealed by Duan, et al, who found that water quality in the regions with rapid economic development was relatively poor in Yangtze River Basin due to the discharge of pollutants such as $\text{NH}_3\text{-N}$ and COD_{Mn} from industrial activities (Weili et al. 2018). In addition, significantly positive correlation between COD_{Mn} and precipitation was observed ($r=0.2737$, $p<0.05$), which further confirmed the speculation that COD_{Mn} in the Yangtze River Basin originated from non-point source proposed in Section 3.1. As for TP, it exhibited a positive correlation with total water resource ($r=0.4303$, $p<0.05$). There would be more particulate phosphorus adsorbed by the suspended sediment existing in the large volume water, therefore the correlation further proved the speculation that the main form of TP was particulate phosphorus in Yangtze River Basin in section 3.1.

Additionally, positive correlation was observed between $\text{NH}_3\text{-N}$ and the number of reservoirs ($r=0.5682$, $p<0.05$). It was reported that the operation process of the reservoirs could greatly alter the discharge and sediment loads (Guo et al. 2011, Li et al. 2021a). And suspended sediment is an important adsorption medium for pollutants in river catchments (Wu et al. 2021b). Thus, the building of reservoirs could decrease the concentration of $\text{NH}_3\text{-N}$, TP and other nutrients due to the adsorption by suspended matter. These might provide a reasonable explanation for the relationship between $\text{NH}_3\text{-N}$ and the number of reservoirs. This could also be confirmed by the fact that the concentration of $\text{NH}_3\text{-N}$ was lower in the outlet of Three Gorges Dam than that in inlet from 2006 to 2011 (Zhao et al. 2013). However, adsorbed particles of nutrients could also be transformed into dissolved states and released from the solid material again and cause secondary pollution in a long period. Hence, it is essential to consider the release risk of the accumulated pollutants stock when the dam was decommissioned. $\text{NH}_3\text{-N}$ was negatively associated with I in WEPM ($r=-0.2193$, $p<0.05$), which demonstrated that increasing government financed investments in environment recent years have contributed much to the decrease of the concentration of $\text{NH}_3\text{-N}$, which was in highly consistent with the view from Zhou, et al (Zhou et al. 2017).

In China's inland surface water, COD_{Mn} and $\text{NH}_3\text{-N}$ that indicating concentration of organic matter and nitrogen were the major types of pollutants(You et al. 2019). Thus, it is quite significant to detect the drivers of the COD_{Mn} and $\text{NH}_3\text{-N}$ spatiotemporal variation in Yangtze River Basin. The total explanation rates of 15 drivers and 103 samples analyzed in RDA reached 50.27%. Moreover, the eigenvalues of ranking axis 1-2 were 0.1182 and 0.0054, and the cumulative explanatory variables were 48.07% and 2.20% respectively. The relationship between water quality indicators and driving factors was highly consistent with the results of the Pearson correlation analysis analyzed above (Figure 5). In the hierarchical segmentation process, tertiary industry (TI), nitrogen fertilizer application rate (N-FAR), phosphate fertilizer application rate (P-FAR) and irrigation area of arable land (IAAL) were detected to be the main divers of COD_{Mn} and $\text{NH}_3\text{-N}$ in Yangtze River Basin, and the contribution rate was 15.92%, 14.65%, 3.46% and 2.84% respectively (Figure 6). From another perspective, anthropogenic activity factors (N-FAR and P-FAR), socioeconomic factors (TI) and land use factors (IAAL) determined COD_{Mn}

and $\text{NH}_3\text{-N}$ in Yangtze River Basin, and their contribution rate were 18.11%, 15.92% and 2.84%, respectively.

Tertiary industry contributed 15.92% explanation rate in the temporal variation of COD_{Mn} and $\text{NH}_3\text{-N}$, which revealed the strong correlation between pollutants and socioeconomic factors in Yangtze River Basin. Rapid economic development and urbanization caused the significant increase discharge of the various pollutants and thus threaten the water environment and ecological security. Duan, et al analyzed the relationship between water quality data (COD_{Mn} , $\text{NH}_3\text{-N}$ and DO) and drivers (GDP and precipitation, etc.) in a qualitative perspective by stacking the elements in one figure. And they found that water quality in the GDP and population concentrated area such as the Yangtze River Delta Economic Zone, etc. was relatively poor, attributed to the discharge from the industrial and household waste-water (Weili et al. 2018). In this study, it was concluded that the influence extent of socioeconomic factors on water quality in a quantitative perspective. When taking the results above into account, it is necessary to regulate the economic development speed and adjust the industry structure in order to further control the concentration of COD_{Mn} and $\text{NH}_3\text{-N}$ in Yangtze River. Also, effective politics should be adopted to support for the surrounding area development so as to disperse population pressure concentrated in this area.

Combined with the result of Pearson correlation analysis, COD_{Mn} showed higher association with land use factors ($r=-0.1990$, $p<0.05$) than $\text{NH}_3\text{-N}$ ($p>0.05$), similar to the results from Wu, at al (Wu et al. 2021a). However, the negative correlation between the main driver (P-FAR, N-FAR and IAAL) and the water quality parameters (COD_{Mn} and $\text{NH}_3\text{-N}$) is notable for the opposite appearance as predicted. Several studies reported the agriculture (Morrice et al. 2008, Nielsen et al. 2012, Wu et al. 2021a) and N fertilizers (Zhou et al. 2021) was the main stressor of nitrogen related indicators including dissolved inorganic nitrogen (DIN), TN, ammonia ($\text{NH}_3\text{-N}$) positively. But it was also demonstrated that the concentration of $\text{NH}_3\text{-N}$ negatively correlated with agriculture (Sliva & Williams 2001, You et al. 2019). It is unquestionable P-FAR, N-FAR and IAAL were the main drivers that totally explained 18.76% for the temporal evolution of COD_{Mn} and $\text{NH}_3\text{-N}$. The negative relationship with COD_{Mn} and $\text{NH}_3\text{-N}$ was also confirmed both by Pearson correlation analysis and RDA analysis. The mechanism under this relationship needs further exploration. Here, we proposed a possibility that the application of nitrogen and phosphorus fertilizers application might not exceed the demand of actual agriculture and the discharge of them into the water body provide necessary nutrient elements for algae growth, which in turn benefit for the purification of pollutants in waters.

3.4 Main driver detection for spatial heterogeneity in Yangtze River Basin

It has been proposed that natural environment (climate and topography) is important in explaining water quality parameters variation in China inland surface water, while land use and socioeconomic factors seem more prominent in small area (You et al. 2019). Factors may display different influence at different spatial scale. Thus, multiple linear regression was conducted for the influence factors including

meteorological, anthropogenic activity, land use and socioeconomic factors to study the main driving factors of spatial heterogeneity in Yangtze River Basin (Table S2). The results revealed that socioeconomic factors were the main drivers for the spatially distinction of COD_{Mn} ($R^2=0.6358$, $p<0.05$), among which tertiary industry showed relatively significant influence. Actually, tertiary industry has shown significant influence on the dynamic of the concentration of COD_{Mn} in Yangtze River in both spatial and temporal scale. Hence, it is meaningful to regulate the speed of economic growth and facilitate the balanced development of regional tertiary industry in Yangtze River Basin. Anthropogenic activity factors ($p<0.1$, $R^2=0.6833$) explained most spatial heterogeneity of $\text{NH}_3\text{-N}$. Among them, total wastewater discharge and the number of reservoirs had a significant impact. Therefore, controlling the utilization of nitrogen and phosphorus fertilizers, stabilizing the operation of the reservoirs, and controlling the point source discharge of wastewater could be the effective strategies to decrease the concentration of $\text{NH}_3\text{-N}$ in Yangtze River Basin.

The spatial difference of TP in Yangtze River also attributed to anthropogenic activity factors in some degree ($p<0.1$, $R^2=0.7115$) (I in WEPM, N-FAR, P-FAR significantly). It could be concluded that TP mainly came from agricultural sources (Bai et al. 2021), which also confirmed the distribution result of TP in Section 3.2. Therefore, it is crucial to control the agricultural non-point pollution in the water quality management. Additionally, environmental investment was significantly associated with TP control ($r=-0.00025$, $p<0.05$), which indicated that national environmental investment paid dividends for the improving water quality of China (Zhou et al. 2017). However, the pollution of TP caused by imperfect mining facilities would also threaten the surface water environment. Thus, it can be controlled in some degrees through the increasing imports of high-grade foreign phosphate ore resources in the "Belt and Road" cooperation. Additionally, the control of TP pollution should also be conducted by a series of comprehensive measures such as carrying out effective government policies, improving emission standards and developing clean production technologies and so on.

4 Conclusion

In this study, spatial and temporal dynamics of water quality and their driving factors in the Yangtze River Basin were identified using multi-statistical analyses (Pearson correlation, RDA and linear regression). The main water quality parameters ($\text{NH}_3\text{-N}$ and TP) decreased significantly from 2008 to 2020. It was predicted that $\text{NH}_3\text{-N}$ concentration would continue to decrease by using of M-K test and R/S analysis, while COD_{Mn} concentration might continue to increase in the next 13 years, which should be paid more attention. In terms of spatial distribution heterogeneity, the water quality in upstream of Yangtze River is superior to that in the middle and lower reaches.

Anthropogenic activity factors (N-FAR and P-FAR), socioeconomic factors (TI) and land use factors (IAAL) were estimated to be the main drivers of COD_{Mn} and $\text{NH}_3\text{-N}$ concentration variation in temporal evolution. In addition, socioeconomic factors (tertiary industry obviously), anthropogenic activity factors (total water discharge obviously) and anthropogenic activity factors (I in WEPM, N-FAR and P-FAR obviously) were

dominant in explaining the spatial heterogeneity of COD_{Mn}, NH₃-N and TP concentration respectively in Yangtze River Basin. Therefore, it is crucial to regulate industry structure from tertiary industry to primary industry in order to further control concentrations of COD_{Mn} and NH₃-N. Specially, strict management on agricultural non-point pollution should also be carried out for the control of TP. Our results were expected to provide valuable references for water quality management in Yangtze River Basin.

Declarations

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Appendix. Supplementary material

Ethical Approval

Not applicable

Consent to Participate

Not applicable

Consent to Publish

Not applicable

Author Contributions

Conceptualization, methodology, writing-Review and editing were conducted by Shasha Liu. Software, formal analysis and writing-Original draft preparation were performed by Rui Fu. Investigation was conducted by Yun Liu. Visualization was performed by Chengyu Suo. All authors read and approved the final manuscript.

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Competing interests

The authors have no relevant financial or non-financial interests to disclose.

Availability of data and materials

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Figures

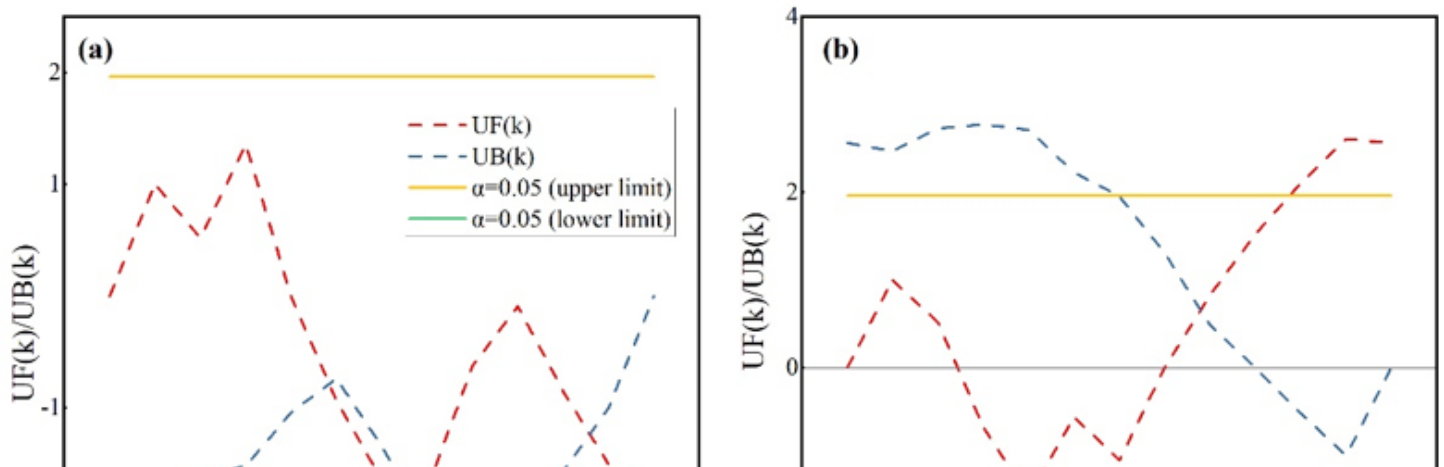


Figure 1

M-K statistic curve of (a) NH₃-N and (b) COD_{Mn} in the Yangtze River Basin. $UF_K > 0$ indicates an upward trend, while $UF_K < 0$ demonstrates a downward trend. The intersection of UF_K and UB_K is the mutation point. It indicates a distinct upward or downward trend when the UF_K exceeds the yellow and green line ($U_{0.05} = \pm 1.96$), respectively.

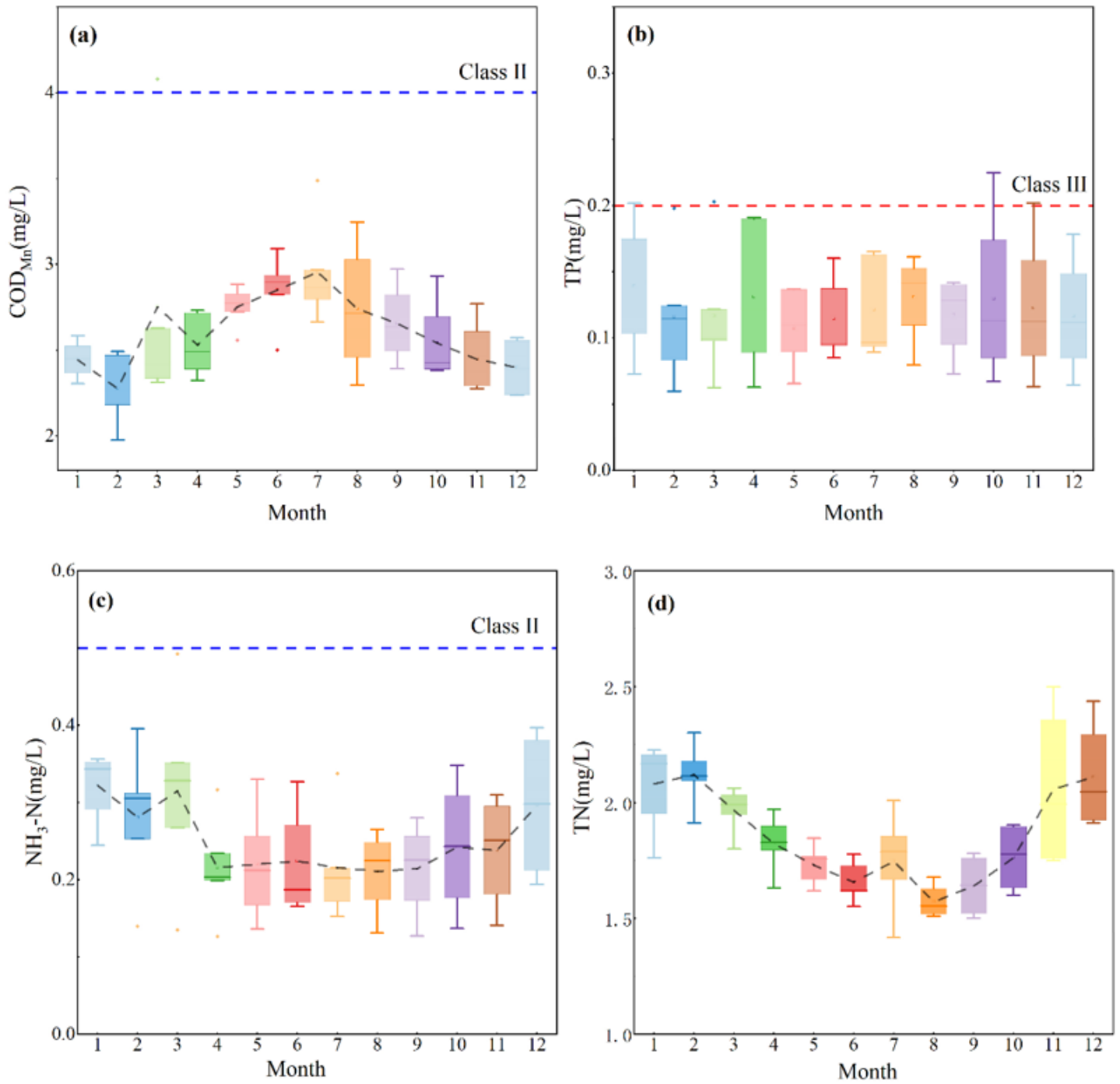


Figure 2

Box plots of monthly dynamic parameters including (a) COD_{Mn}, (b) TP, (c) NH₃-N, and (d) TN from 2016 to 2020 (blue and red dotted line are the standard limitation of class I and class II respectively, according to "Surface Water Environmental Quality Standard" (GB3838-2002)).

Figure 3

The spatial distribution of average values of (a) COD_{Mn}, (b)NH₃-N, and (c)TP in Yangtze River Basin according to from 2016 to 2020. The red dots represent the exceeded sites whose water quality worse than class Ⅲ in GB3838-2002.

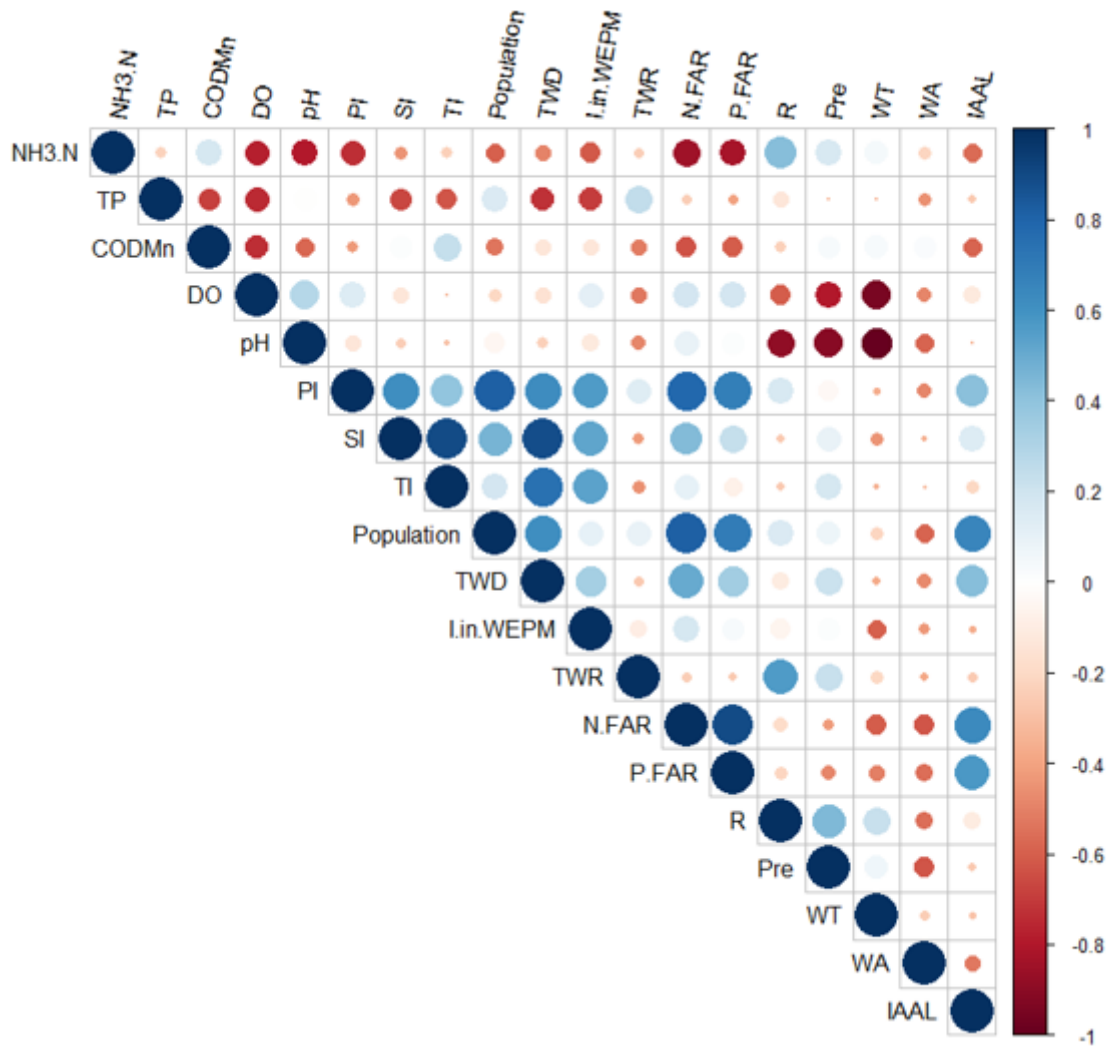


Figure 4

The correlation coefficient graph between water quality parameters and driving factors. The blue dot means positive correlation, while the red dot means the negative correlation. The larger and darker the dot, the stronger the correlation. The driving factors include pH, primary industry (PI), secondary industry (SI), tertiary industry (TI), total wastewater discharge (TWD), investment in water conservancy, environment and public facilities management industry (I in WEPM), total water resources (TWR), nitrogen and phosphate fertilizer application rate (N-FAR and P-FAR respectively), reservoirs (R), precipitation (Pre), water temperature (WT), wetland area (WA), irrigation area of arable land (IAAL).

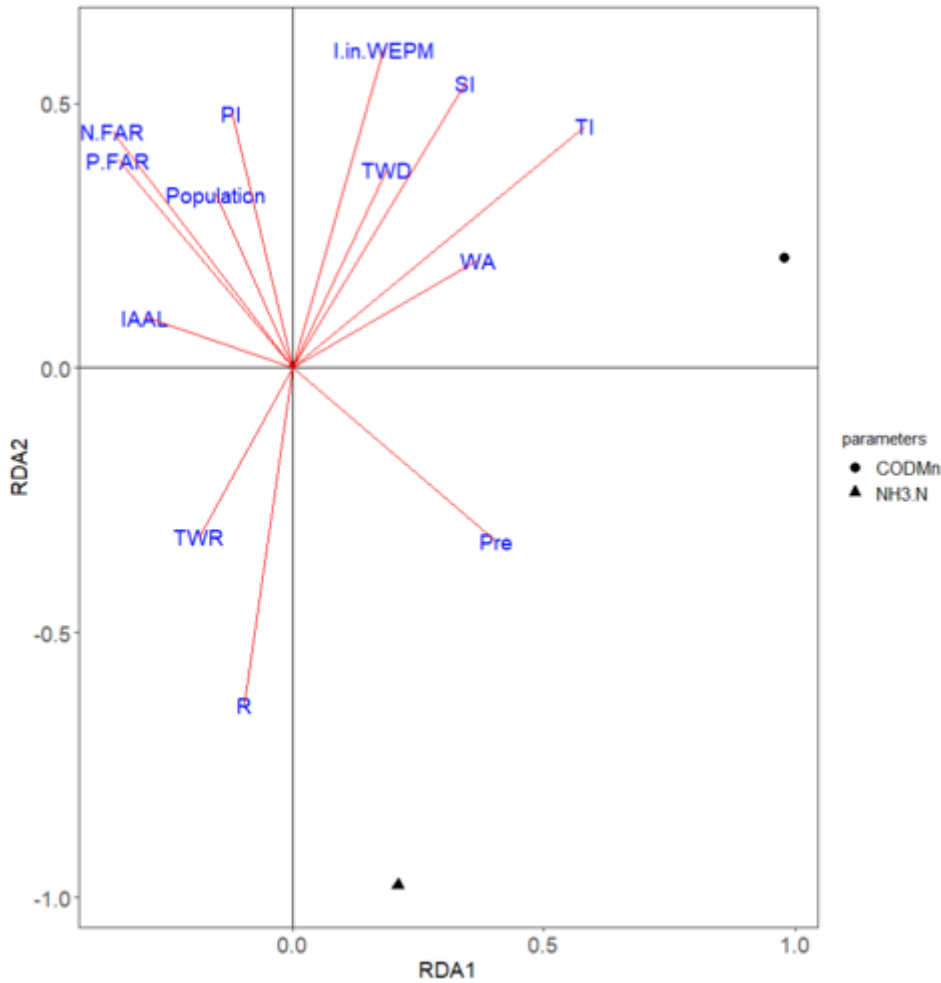


Figure 5

Biplot diagram for RDA analysis between water quality parameters (including COD_{Mn} and $\text{NH}_3\text{-N}$) and driver factors (including primary industry (PI), secondary industry (SI), tertiary industry (TI), total wastewater discharge (TWD), investment in water conservancy, environment and public facilities management industry (I in WEPM), total water resources (TWR), nitrogen and phosphate fertilizer application rate (N-FAR and P-FAR respectively), reservoirs (R), precipitation (Pre), wetland area (WA), irrigation area of arable land (IAAL))

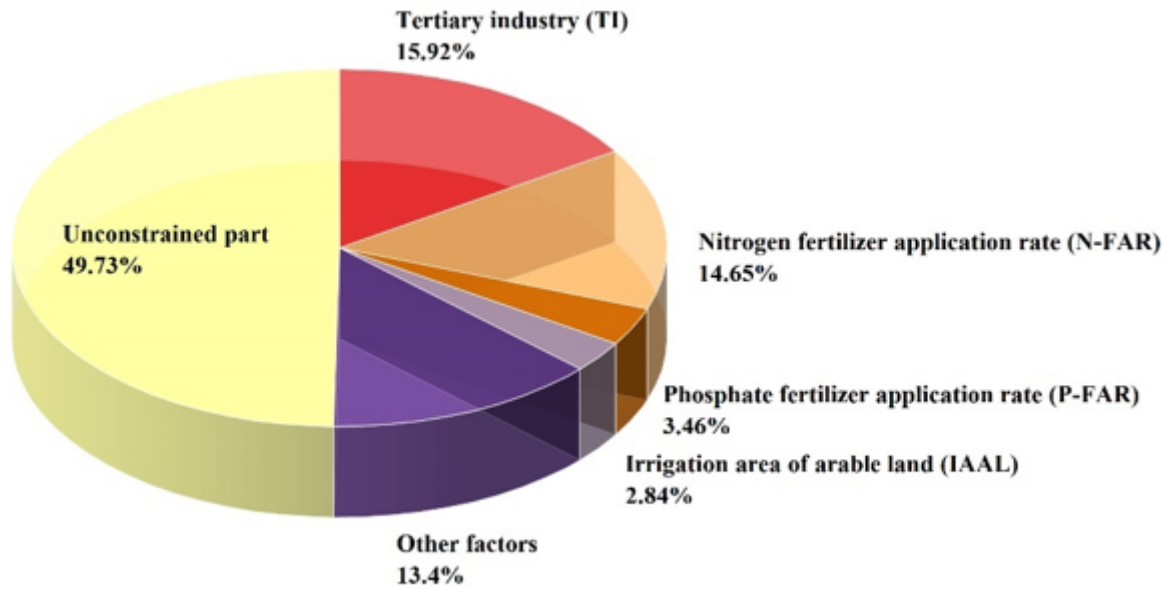


Figure 6

Contribution rate of each driving factor obtained by hierarchical segmentation.

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