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Article

Monitoring Water Quality Parameters Using Sentinel-2 Data: A Case Study in the Weihe River Basin (China)

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Abstract: Based on Sentinel-2 multispectral image data and existing research results, the comprehensive water quality index (CWQI), $\text{NH}_4^+\text{-N}$, and total phosphorus (TP) in the Weihe River and its tributaries were estimated. Furthermore, a verified model was obtained by fitting the regression using the measured and inverted data. The verified model results show that the average relative error of the CWQI is only 9.80%, the goodness of fit of $\text{NH}_4^+\text{-N}$ and TP concentrations is 0.62 and 0.61, respectively, and the average relative errors are 19.40% and 24.70%, respectively. The accuracy of the verified model is relatively high, and it can approximately invert the distribution of the three parameters of the Weihe River and its tributaries. In December 2023, except for the Bahe River between Puhua Town and Sanli Town in Lantian County, most of the water bodies in the Weihe River and its tributaries had good water quality. The study can provide an example of how to monitor water quality information using Sentinel-2 data in similar river basins.



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Keywords: Sentinel-2; Weihe River; water quality; inversion

1. Introduction

Water is one of the most essential natural resources on Earth, sustaining the balance of ecosystems and the sustainable development of human society [1]. With the increasing global population and expanding economic activities, water resources' quality and quantity are facing severe challenges [2]. Particularly, in rapidly urbanizing and industrializing areas, water pollution problems are becoming increasingly severe, posing significant threats to local ecosystems and public health [3]. Therefore, conducting water quality monitoring and research to identify pollution sources and propose effective remediation measures is crucial in current environmental science research [4].

The water quality of any specific region or source can be assessed using physical, chemical, and biological parameters [1]. Threshold values are often established for these parameters to evaluate the quality of the water body. These thresholds help determine whether the water body meets safety and quality standards [5]. With the development of times and progress in science and technology, water quality assessment methods have become increasingly diverse, and water quality assessment systems have become more comprehensive. In the field of fuzzy mathematics theory, Lu et al. [6] used the entropy weight method for fuzzy comprehensive evaluation to assess the water quality of the Wei River, and the results showed that this evaluation method was effective. In the field

of artificial neural networks (ANNs), Liu et al. [7] established an effective and stable water quality prediction model using a large amount of data obtained from water quality monitoring experiments. Jiang et al. [8] developed an ANN model for the eutrophication assessment of lakes in eastern China, which proved to be highly applicable to the study area. Research by Palani and Singh demonstrated that the ANN model could be used as a tool for calculating water quality parameters and could provide simulated data required by the model for areas where measurement data are difficult to obtain [9,10]. Additionally, there are other methods for water quality assessment, such as projection pursuit [11–14]. Overall, water quality assessment methods are becoming more diversified, and the complexity of water quality assessment issues is gradually increasing [15]. In practical research, the appropriate evaluation method should be selected based on specific situations. Domestic and international scholars have provided a wealth of research results on water quality assessment methods and indicators.

The single-factor evaluation method assesses whether the water quality meets the standards by comparing single water quality indicators with standard values. However, due to its partial and pessimistic results, it cannot comprehensively reflect the overall water quality and tends to show an over-protection state [16]. Therefore, it is often used in combination with other comprehensive evaluation methods. Comprehensive index evaluation methods use weighted averages, indices, and other calculation methods to combine independent monitoring results of multiple pollutants, reducing a large number of parameters and providing a relatively simple and understandable numerical value that is categorized into several levels to distinguish water quality grades [17].

In 1965, Horton et al. [18] first proposed the Horton water quality index (WQI) by selecting ten commonly used water quality parameters (such as dissolved oxygen, pH value, fecal coliforms, etc.) to calculate the water quality index. Brown et al. [19] later proposed the Brown water quality index (Brown WQI), which is similar to the Horton Index but includes nine parameters with weights determined by expert ratings, introducing subjectivity. In 1974, Nemerow proposed the Nemerow pollution index (NPI), selecting 14 parameters to calculate the water quality index based on the water body's usage, highlighting the most severe pollutants, and this method has been widely applied [20]. Ross, summarizing previous methods, proposed a simplified water quality index calculation method by selecting four key parameters (such as BOD, $\text{NH}_4^+\text{-N}$, dissolved oxygen, and suspended solids) for evaluation, simplifying the calculation process [21]. Sargaonkar et al. [22] developed the comprehensive pollution index evaluation method, which does not consider the weights of the evaluated factors and uses the arithmetic mean of the standard indices of various factors to calculate the comprehensive pollution index. The Oregon water quality index (OWQI) uses eight parameters (such as temperature, dissolved oxygen, BOD, etc.) and is mainly used for recreational, swimming, and fishing purposes [23]. The comprehensive water quality index (CWQI) evaluates water quality through three aspects: scope, frequency, and amplitude, making it scientifically reasonable and widely applicable for evaluating drinking water quality in Canada and by the United Nations Environment Programme (UNEP) [24,25]. Farzadkia et al. [26] evaluated the water quality of the Yamchi Dam watershed using the CWQI model, finding that aquaculture wastewater and urban industrial wastewater are the main sources of pollution, with total coliforms in drinking water and total suspended solids in irrigation water being the most severe issues. John-Mark Davies used the CWQI model to analyze a river in northern USA, and the results indicated that the CWQI values reflected variations in sample collection [27].

The Weihe River, the largest tributary of the Yellow River, serves as a crucial water source for the Guanzhong Plain, the economic center of western China. Its significance in water resource management and development within the Yellow River Basin cannot be overstated, as it holds strategic importance for regional economic growth and the Western Development Initiative [28]. However, rapid industrialization and urbanization have exacerbated water quality issues in the Weihe River, posing severe challenges to communities' livelihoods, productivity, and ecological environments along its banks. The

construction of 32 water diversion projects along the Weihe River in the Guanzhong region has further exacerbated pollution problems; particularly, organic pollutant levels have increased [29]. In recent years, the sharp decrease in runoff in the Yellow River Basin has drawn significant attention, indicating significant changes in the hydro-ecological system of the Weihe River, which in turn constrains economic development in the Guanzhong region [30]. Therefore, accurately understanding the water quality status is crucial for the residents' lives and economic growth in the Weihe River Basin, and it can also provide reference information for river water quality management [31].

Traditional water quality studies primarily obtain water quality data through field sampling and laboratory analysis, enabling the calculation of water quality indices using water quality assessment methods. Although this method yields high precision, its coverage is limited and fails to reflect the overall conditions of water bodies comprehensively. With technological advancements, the application of remote sensing data has addressed this issue by enabling the large-scale acquisition of land cover information. Combining remote sensing data with field measurements facilitates the comprehensive monitoring of water quality across water bodies. Scholars worldwide have conducted extensive research in this area, yielding fruitful results. For instance, Thiemann et al. [32] established a linear regression inversion model using measured chlorophyll-a data and remote sensing data to analyze and evaluate the eutrophication status of Lake Mecklenburg in Germany. In 2007, Alparslan et al. [33] utilized Landsat-7 ETM satellite data to analyze the water quality of the Omerli Dam, estimating suspended solids, transparency, and total phosphorus with high correlation. Using Sentinel-2 satellite images, Zhang et al. [34] successfully tracked the spatial distribution of water quality parameters (CODM, TP, and TN) in seven major rivers in Zhejiang Province, revealing the specific locations of polluted areas. Zhao et al. [35] used SPOT5 remote sensing data to quantitatively retrieve water quality parameters for the Weihe River in Shaanxi Province through modeling with multiple linear regression and neural networks, achieving favorable results. Shi et al. [36] used Sentinel-2 imagery and water quality data to develop models that analyze the spatial distribution of total phosphorus and $\text{NH}_4^+\text{-N}$ in the downstream and nearshore areas of the Huaihe River Basin. Other researchers have also conducted related studies on water quality parameters such as chlorophyll concentration [37–40], total suspended solids [37,41], and total phosphorus [33] based on remote sensing and field data, making significant contributions to water quality remote sensing monitoring.

Research on monitoring chlorophyll-a concentration, total suspended solids (TSSs), and turbidity in water bodies using remote sensing technology is relatively mature. However, studies on $\text{NH}_4^+\text{-N}$ and total phosphorus (TP) are still insufficient. The application of composite indices is also limited. Building on previous research [25,26,42], this paper will use Sentinel-2 multispectral remote sensing imagery to retrieve and verify the CWQI, $\text{NH}_4^+\text{-N}$, and TP concentrations in the Weihe River. The aim is to obtain verification models and results suitable for the Weihe River Basin, providing a reference for water quality monitoring in the Weihe River.

2. Materials and Methods

2.1. Study Area

The Weihe River originates from Mount Niushoushan in Weiyuan County, Dingxi City, Gansu Province. It traverses eastern Gansu and central Shaanxi, flowing mainly through regions such as Tianshui in Gansu, and Baoji, Xianyang, Xi'an, and Weinan in Shaanxi, before joining the Yellow River at Tongguan County, Weinan City. The Weihe River's main stem spans a length of 818 km, covering a watershed area of 134,700 square kilometers [43,44]. The study area lies between east longitude 107° E – 110° E and north latitude 33° N – 35° N , encompassing the main stem of the Weihe River, as well as its tributaries such as the Heihe River, Laohe River, and Bahe River (Figure 1).

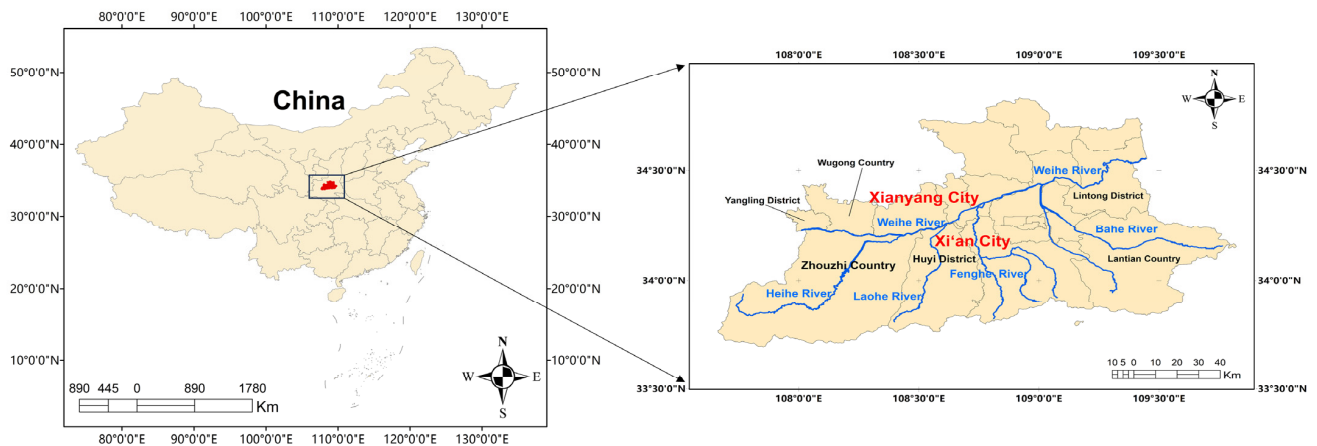


Figure 1. The distribution map of Xi'an City, Xianyang City, and the Weihe River and its tributaries.

2.2. Data

2.2.1. December 2023 Sentinel-2 Multispectral Imagery

This study selected 6 scenes of Sentinel-2A Level-2A imagery from 4 December 2023, with tile IDs 48SYD, 49SBU, 49SCU, 48SYC, 49SBT, and 49SCT. The corresponding cloud cover for each image is 4.7%, 3.0%, 2.5%, 0.7%, 1.2%, and 1.0%, respectively. This product does not require radiometric calibration or atmospheric correction and can be used directly. The Sentinel constellation (Sentinel-2A and 2B polar-orbiting satellites) was jointly developed by the European Commission and the European Space Agency (ESA) to meet the operational needs of the Copernicus programme [45] (https://www.copernicus.eu/sites/default/files/documents/Copernicus_Programme_v2.pdf, accessed on 27 July 2024). The two Sentinel-2 satellites operate in a complementary manner (<https://sentiwiki.copernicus.eu/web/s2-mission>, accessed on 27 July 2024), forming an observation system with a five-day repeat cycle. This short revisit period allows Sentinel-2 to capture changes in the Earth's surface in a more timely and comprehensive manner, which contributes to reducing monitoring costs and responding to emergencies and natural disasters. They are equipped with Multispectral Instruments (MSIs), including nine visible and near-infrared spectral bands [36]. The data encompass three resolution bands: 10 m, 20 m, and 60 m. These data are available for free access through the European Space Agency (<https://browser.dataspace.copernicus.eu/>, accessed on 13 January 2024) [46].

2.2.2. Construction of Water Quality Parameter Inversion Models

After downloading the data, cloud masking will be performed on the images, and the river vector files of the Weihe River and its tributaries will be used for land masking. Once the river channels are obtained, it is worth considering that the water bodies within the channels may not cover the entire river. Therefore, by calculating the normalized difference water index (NDWI) and using the threshold method, the water bodies from the river channels are extracted. Figure 2 shows the water body extraction of the Weihe River and its tributaries.

The previous research [42] established inversion models for the Yi River and Shu River in the Huai River system in China, using data from all periods of the year. Additionally, it estimated the concentrations during the dry season, wet season, and normal flow period, and achieved good results. This study references it and selects an inversion model for the 10 m resolution B4 (red band) as follows:

$$\text{CWQI} = -337.06 \times \text{B4} + 112.21 \quad (1)$$

$$\text{NH}_4^+\text{-N} = 11.17 \times \text{B4} - 0.46 \quad (2)$$

$$\text{TP} = 0.64 \times \text{B4} - 0.027 \quad (3)$$

The inversion model is the model established in the previous research [42], and in this study, the first consideration is whether the model can be applied to the water conditions of the Weihe River, and the second is to establish a model based on it that can be applied to the water conditions of the Weihe River (known as the verified model).

The formula for the NDWI [47] is as follows:

$$\text{NDWI} = (B3 - B8)/(B3 + B8) \quad (4)$$

In the formula, B3 represents the green band (GREEN) of Sentinel-2 data, and B8 represents the near-infrared band (NIR) of Sentinel-2 data. A threshold of 0 is selected for NDWI, with values greater than 0 considered as water bodies.

Using Equations (1)–(3), the values of CWQI, $\text{NH}_4^+\text{-N}$, and TP at various measured cross-sectional locations can be calculated as inversion values. These values will be used to compare and fit regressions to the measured data to build a verified model. During the calculation process, the reflectance values of the bands need to be multiplied by 0.0001 before being used in the calculations.

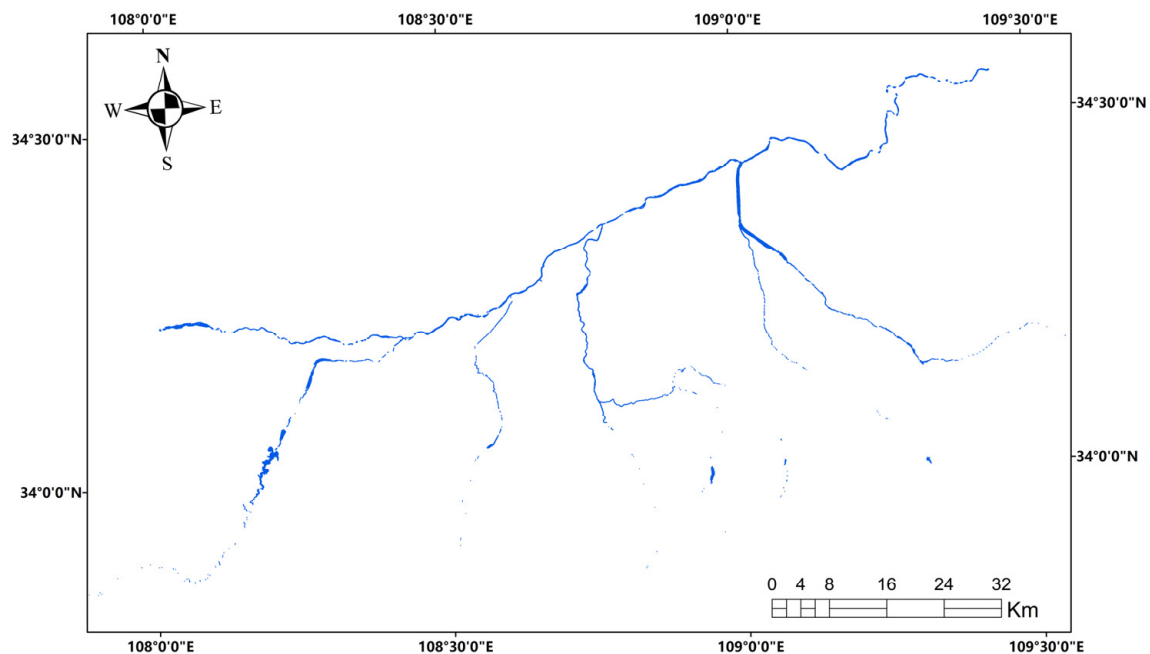


Figure 2. Water body distribution of the Weihe River and its tributaries in December 2023.

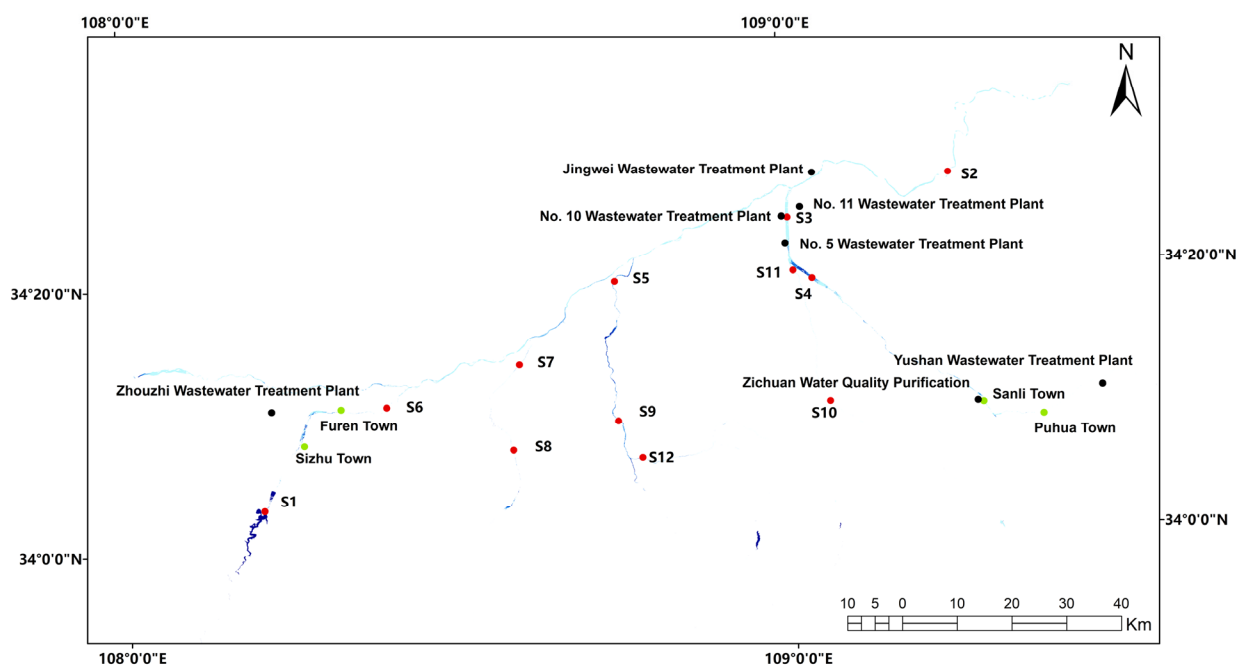
2.2.3. Water Quality Categories of Measured Points and Inverted CWQI in December 2023

Figure 3 shows the distribution of the measured sections, including Furen Town, Sizhu Town, Puhua Town, Sanli Town, and multiple sewage treatment plants. The measured sections comprise 12 points located on the main stream and tributaries of the Weihe River. Measured water quality categories (S1–S12), $\text{NH}_4^+\text{-N}$ values for the 8 measurement points, and TP values for the 8 measurement points were obtained from the Xi'an Ecology and Environment Bureau's report on the state of the water environment quality in Xi'an for the month of December 2023 and the period from January to December, and the document provided the average values for the month of December.

Table 1 provides the CWQI values calculated by the inversion model and the corresponding water quality categories for the matching locations.

Table 1. Measured water body categories and inverted CWQI.

Locations	S1	S2	S3	S4	S5	S6
categories	II	II	III	II	II	I
CWQI	72.20	55.18	49.31	64.01	62.90	58.42
Locations	S7	S8	S9	S10	S11	S12
categories	II	II	III	II	III	III
CWQI	62.25	62.80	63.88	52.35	46.58	49.65

**Figure 3.** Locations of measured sections (S1–S12), towns, and sewage treatment plants (red points indicate measured sections, green points indicate small towns, and black points indicate sewage treatment plants).

This study will establish a brief correspondence between water quality categories and CWQIs for use in subsequent comparisons and fitted regressions (Table 2). In this correspondence, Class I water corresponds to excellent water quality (CWQI value of 95), Class II water corresponds to good water quality (CWQI value of 87.5), Class III water corresponds to fair water quality (CWQI value of 72.5), Class IV water corresponds to poor water quality (CWQI value of 57.5), and Class V water corresponds to very poor water quality (CWQI value of 49). The median value is taken as the representative for the intermediate three categories. For Class I and Class V, the minimum and maximum values are taken as representatives, respectively. As a result, a simple relationship is established between CWQI and water quality categories.

Table 2. Explanation of CWQI classifications [42].

CWQI Value	Water Quality Category	Explanation
≥ 95	Excellent (I)	Water quality protected
80–94	Good (II)	Water quality protected, only occasionally subject to minor pollution
65–79	Fair (III)	Water quality generally protected, but occasionally subject to pollution
50–64	Marginal (IV)	Water quality frequently polluted
≤ 49	Poor (V)	The water quality is consistently heavily polluted

2.2.4. TP and $\text{NH}_4^+\text{-N}$ Concentrations at Measured Points in December 2023

The measured and inverted $\text{NH}_4^+\text{-N}$ and TP values for the six measurement sites are given in Tables 3 and 4, respectively.

Table 3. Measured and inverted $\text{NH}_4^+\text{-N}$ (mg/L).

Locations	S1	S3	S4	S5
Measured	0.29	0.31	0.17	0.15
Inverted	1.43	1.63	1.14	1.11
Locations	S6	S8	S10	S11
Measured	0.12	0.13	0.22	0.17
Inverted	1.33	1.18	1.53	1.29

Table 4. Measured and inverted TP (mg/L).

Locations	S2	S3	S4	S5
Measured	0.066	0.054	0.032	0.068
Inverted	0.081	0.092	0.064	0.074
Locations	S7	S8	S10	S11
Measured	0.040	0.020	0.080	0.080
Inverted	0.068	0.067	0.086	0.097

2.3. Method

The study applied the model established by previous authors to obtain the values of CWQI, $\text{NH}_4^+\text{-N}$, and TP (called inverted values) for the B4 band at each measurement point. However, it does not mean that these values can better reflect the water quality condition of the Weihe River and its tributaries, so they need to be further compared, modelled, and validated using measured data. The modeling process used SPSS statistical software (the online version, which can be accessed via the web page, <https://spssau.com/index.html>, accessed on 28 April 2024) to perform a linear regression on the inverted and measured values, thus establishing an inversion model based on measured data for the three parameters (called the verified model). The results were also plotted with the help of MATLAB-R2022a and ARCGIS-10.8 software.

3. Results

3.1. Comparison and Verified Model

In Figure 4, the CWQI values directly inverted from the measured model are all lower than the measured values, with a significant error. The average relative error is 29.70%, indicating that the model's direct calculation tends to underestimate the water quality of the Weihe River and its tributaries.

Figures 5 and 6 show that the concentrations of $\text{NH}_4^+\text{-N}$ and TP obtained directly from the model inversion are higher than the measured concentrations. This indicates an overestimation of these two parameters in the Weihe River and its tributaries. The average relative error of TP concentrations across the cross-sections is as high as 66.7%, and the inverted concentration of $\text{NH}_4^+\text{-N}$ is nearly 10 times higher than the measured value.

Given the huge difference between the estimated and measured values of the inversion model, this study will fit a regression between the two, with the aim of establishing an inversion model suitable for the Weihe River and its tributaries (verified model).

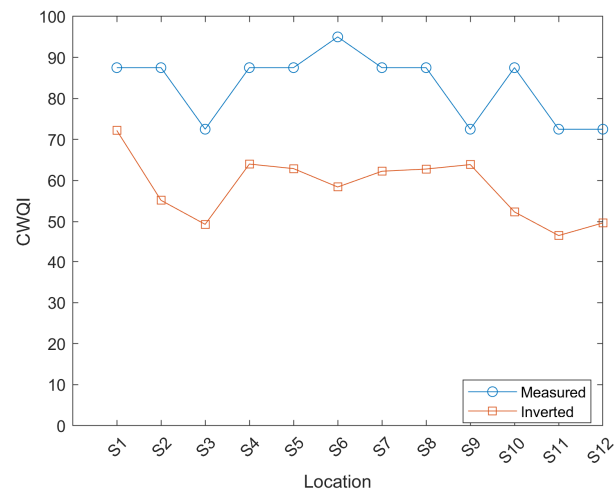


Figure 4. Line chart of measured and inverted CWQI values.

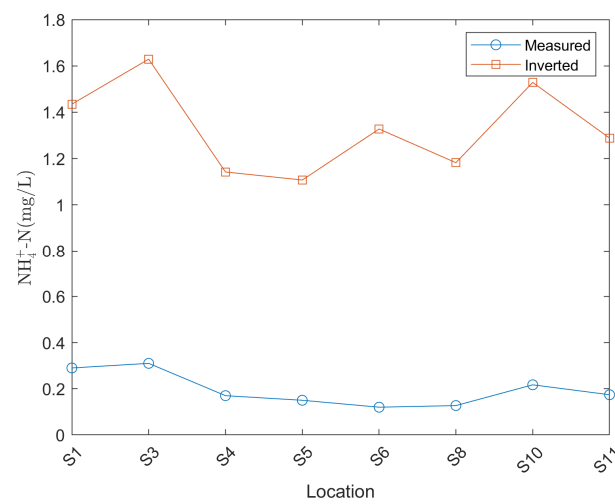


Figure 5. Line chart of measured and inverted $\text{NH}_4^+\text{-N}$ concentrations.

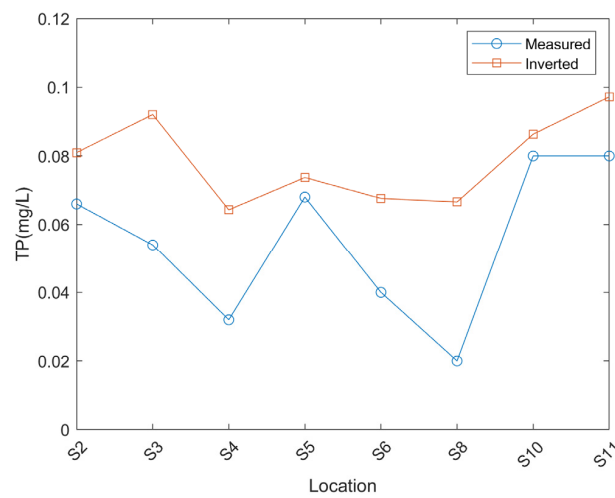


Figure 6. Line chart of measured and inverted TP concentrations.

3.1.1. CWQI Verified Model

For CWQI, data from sections S1–S7 were selected for multiple linear regression, and data from sections S8–S12 were used for validation. The regression equation and optimal model obtained after regression is as follows:

$$y = 0.4845x + 57.06 \quad (5)$$

$$\text{CWQI} = -163.31 \times B_4 + 111.43 \quad (6)$$

The measured and verified CWQI values for sections S8–S12 are shown in Table 5.

Table 5. Measured and verified CWQI values.

Locations	S8	S9	S10	S11	S12
categories	II	III	II	III	III
CWQI	87.49 (II)	88.01 (II)	82.43 (II)	79.63 (III)	81.12 (II)

The results (Figure 7) indicate that the inverted CWQI values from the verified model for sections S8–S12 agree with the measured CWQI values, with an average relative error of 9.80%. The model error is relatively small.

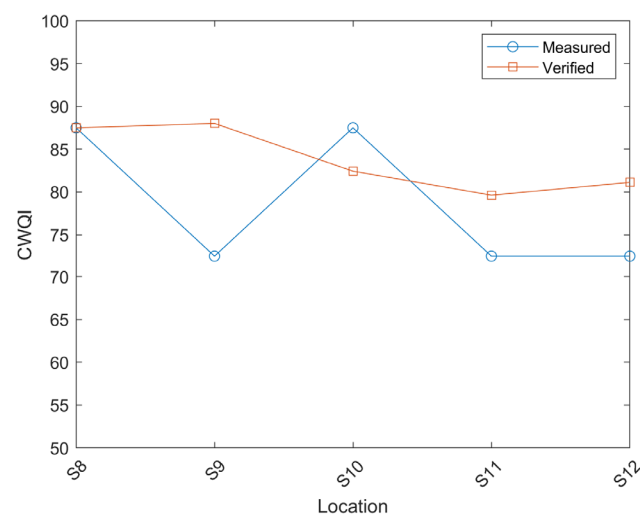


Figure 7. Line chart of measured and verified CWQI for sections S8–S12.

3.1.2. $\text{NH}_4^+\text{-N}$ Verified Model

For $\text{NH}_4^+\text{-N}$, the measured and inverted values in Table 3 were subjected to multiple linear regression and the optimal model obtained is shown in Figure 8.

$$\text{NH}_4^+\text{-N} = 3.35 \times B_4 - 0.34 \quad (7)$$

The goodness of fit for the $\text{NH}_4^+\text{-N}$ verified model is 0.62, indicating a good fit. The F-test result for $\text{NH}_4^+\text{-N}$ was $F = 9.802$, $p = 0.020 < 0.05$. The measured and verified values for each section are shown in Table 6.

Table 6. Measured and verified $\text{NH}_4^+\text{-N}$ (mg/L).

Locations	S1	S3	S4	S5
Measured	0.29	0.31	0.17	0.15
verified	0.23	0.28	0.14	0.13
Locations	S6	S8	S10	S11
Measured	0.12	0.13	0.22	0.17
verified	0.19	0.15	0.25	0.18

The average relative error between the measured and verified $\text{NH}_4^+\text{-N}$ values for each section is 19.40%, which is below 20%, indicating that the model is highly accurate.

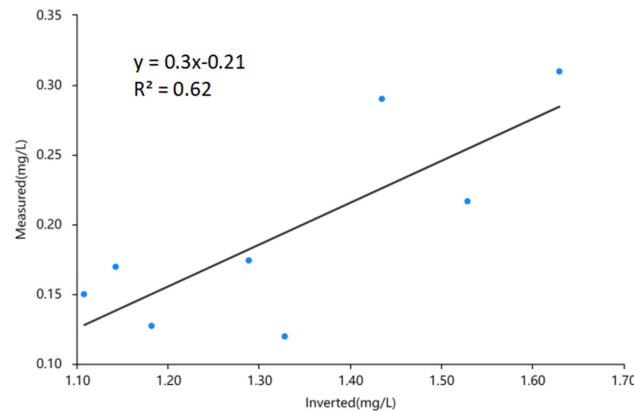


Figure 8. $\text{NH}_4^+\text{-N}$ regression results.

3.1.3. TP Verified Model

For TP, the measured and inverted values in Table 4 were subjected to multiple linear regression and the optimal model obtained is shown in Figure 9.

$$\text{TP} = 0.89 \times \text{B4} - 0.093 \tag{8}$$

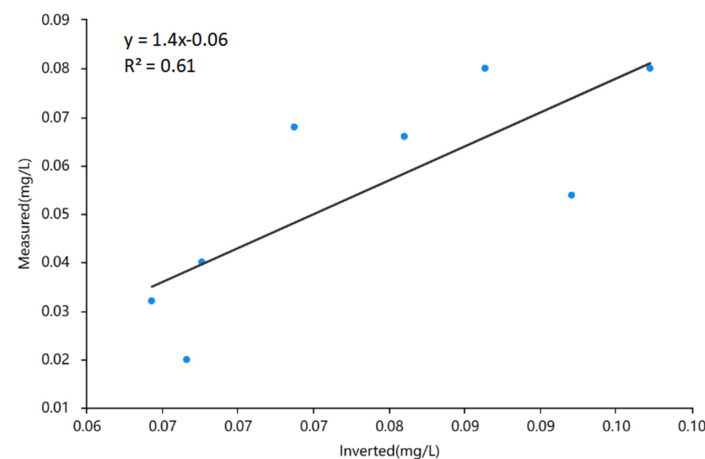


Figure 9. TP regression results.

The goodness of fit for the TP verified model is 0.61, indicating a good fit. The F-test result for TP was $F = 9.220$, $p = 0.023 < 0.05$. The measured and verified values for each section are shown in Table 7.

The average relative error between the measured and verified TP values for each section is 24.70%, which is below 25%, indicating that the model accuracy is highly accurate.

Table 7. Measured and verified TP (mg/L).

Locations	S2	S3	S4	S5
Measured	0.066	0.054	0.032	0.068
verified	0.058	0.074	0.035	0.048
Locations	S7	S8	S10	S11
Measured	0.040	0.020	0.080	0.080
verified	0.040	0.038	0.066	0.081

3.2. Verified Model Inversion Results

The error analyses and goodness of fit of the three models showed that the verified models could effectively estimate CWQI, $\text{NH}_4^+\text{-N}$, and TP in the Weihe River and its tributaries.

3.2.1. Estimated CWQI Results for December 2023

Figure 10 shows that the CWQI values estimated by the inversion model for the Weihe River Basin are generally low, mainly ranging mostly between 35 and 70. According to the CWQI classification, the water quality of the Weihe River is categorized as fair or below. However, the actual situation indicates that after long-term management, the water bodies in the Weihe River and its tributaries have underwent significant improvement, leading to a substantial enhancement in water quality [48]. Therefore, the water quality category in the Weihe River Basin does not align with the estimated results.

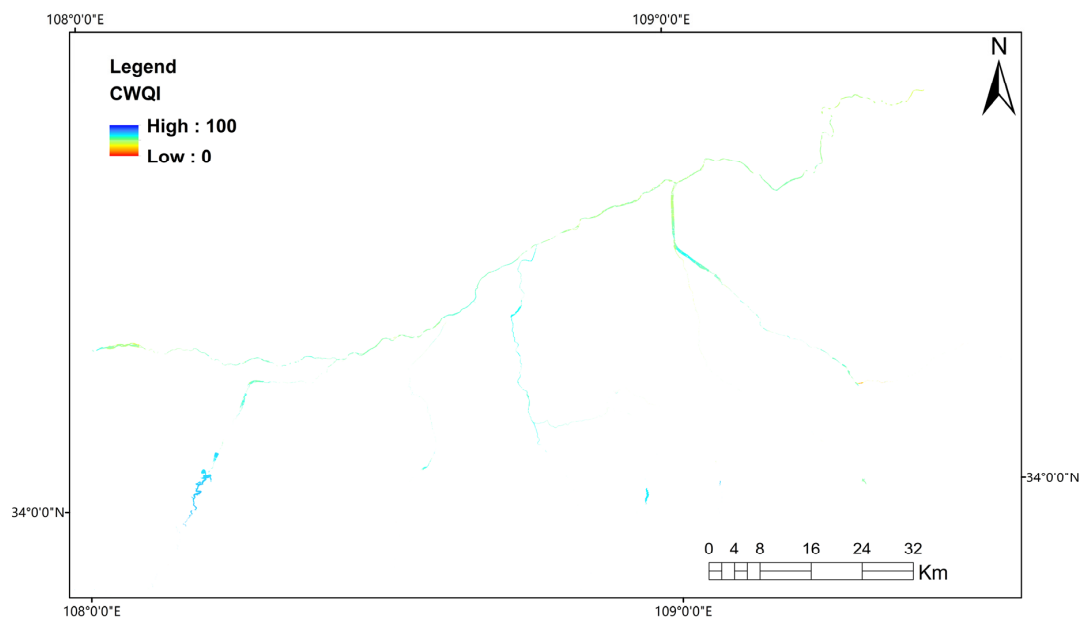


Figure 10. Distribution of CWQI for the Weihe River and its tributaries in December 2023 estimated by the inversion model.

The CWQI distribution for December 2023 was obtained from the CWQI verified model estimates. Observing Figure 11, we can see that the CWQI for December generally falls within the range of 70–90. The water quality of the main stream of the Weihe River is poorer than that of its tributaries. This is because before 2015, most of the sewage outlets along the coast flowed into the Weihe River, which carried 80% of the sewage and wastewater discharge [48]. Although water quality improvement measures have been implemented since 2015, and the effects are relatively significant, there may still be some pollution. Tributaries generally have better water quality, but certain areas may be affected by nearby sewage treatment plants, resulting in relatively poor water quality. For example, the Heihe River between Furen Town and Sizhu Town may receive discharge from the nearby Zhouzhi sewage treatment plant, and the Bahe River between Puhua Town and Sanli Town in Lantian County may be affected by sewage stations such as the Yushan sewage treatment plant, with the water quality ranging from 50 to 70. The CWQI of water bodies in each tributary segment is generally worse than those further away from the Weihe River segment.

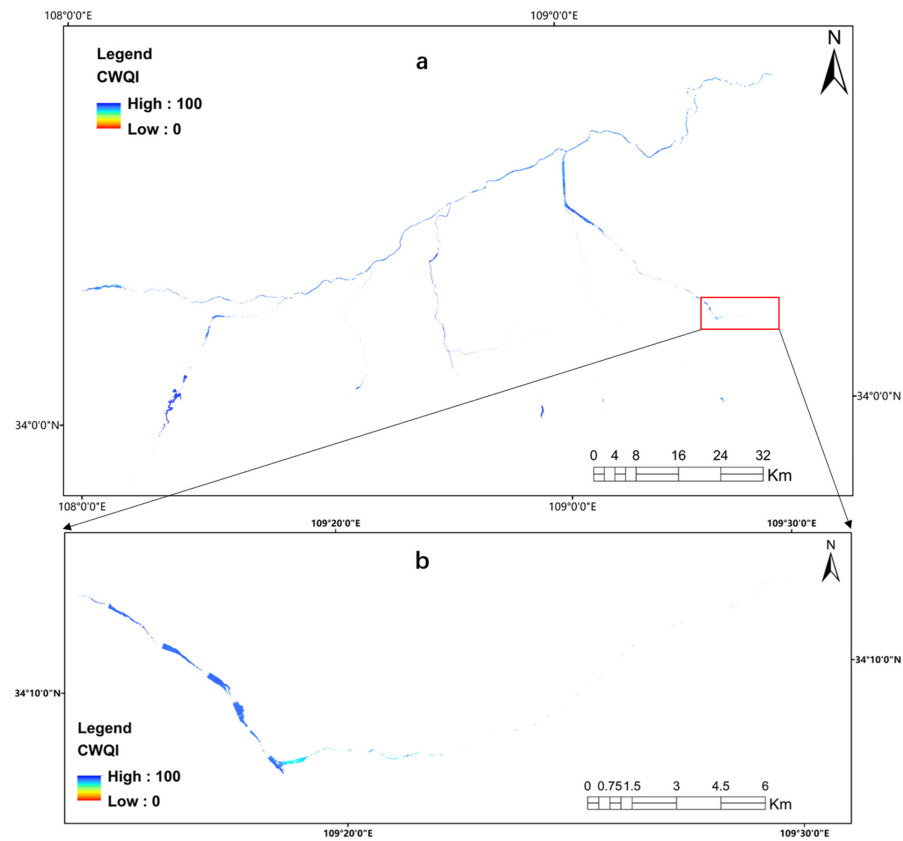


Figure 11. Distribution of CWQI for the Weihe River and its tributaries in December 2023 obtained from the verified model (“a” represents the overall distribution of the river, and “b” represents the river segment in the area of Lantian County).

3.2.2. Estimated NH_4^+ -N Results for December 2023

The NH_4^+ -N inversion results (Figure 12) indicate that the NH_4^+ -N concentration in the study area is generally high, ranging from 0 to 3 mg/L, with significant deviations from the measured concentrations. The distribution of NH_4^+ -N concentration was obtained from the verified model. The goodness of fit for the verified model is 0.62, and it passed the significance test at the 95% confidence level.

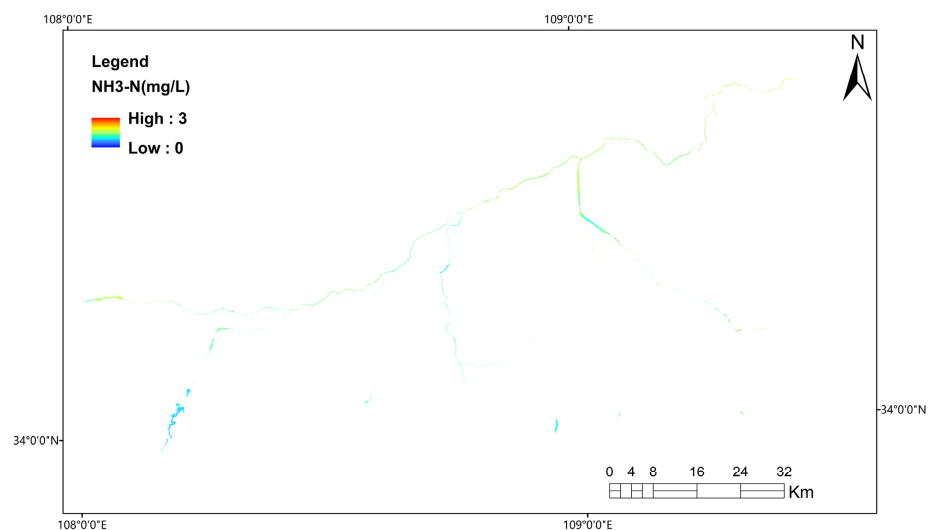


Figure 12. Distribution of NH_4^+ -N for the Weihe River and its tributaries in December 2023 obtained from the inversion model.

In December 2023, the verified model estimated $\text{NH}_4^+\text{-N}$ concentrations (Figure 13) for the mainstream of the Weihe River range between 0.10 and 0.40 mg/L. The $\text{NH}_4^+\text{-N}$ concentrations in the Heihe River and Bahe River segments entering the Weihe River are higher than those further away from the main stream, ranging from 0.20 to 0.40 mg/L. The $\text{NH}_4^+\text{-N}$ concentration in the Jinpen Reservoir (S1) of the Heihe River is the lowest in the entire study area, mostly below 0.10 mg/L. However, in the area of Lantian County, the $\text{NH}_4^+\text{-N}$ concentration in the Bahe River between Puhua Town and Sanli Town is relatively high, ranging from 0.50 to 1.00 mg/L.

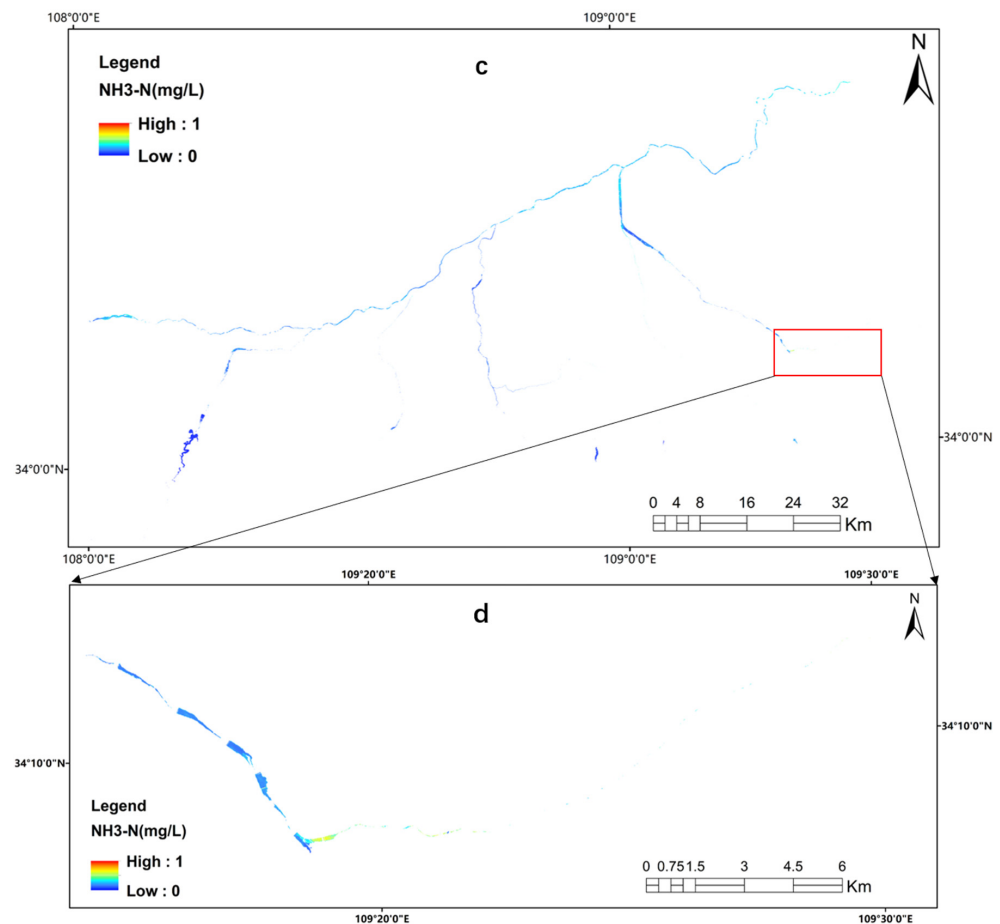


Figure 13. Distribution of $\text{NH}_4^+\text{-N}$ for the Weihe River and its tributaries in December 2023 obtained from the verified model (“c” represents the overall distribution of the river, and “d” represents the river segment in the area of Lantian County).

3.2.3. Estimated TP Results for December 2023

The TP inversion results (Figure 14) show that the TP concentration in the study area is generally close to the measured values but slightly higher, ranging from 0.00 to 0.12 mg/L.

After fitting a regression through measured and inverted data, the goodness of fit for the verified model is 0.61, and it passed the significance test at the 95% confidence level. The distribution of TP concentration (Figure 15) inverted by the verified model reflects that the concentration is higher in the mainstream of the Weihe River than in its tributaries, ranging from 0.04 to 0.08 mg/L. There are noticeable high values of TP concentrations in the Heihe River and Bahe River segments near the Weihe River, ranging from 0.04 to 0.08 mg/L, with higher concentrations in the Bahe River segment near the Weihe River. The TP concentration in the Bahe River water in Lantian County is mostly higher than 0.08 mg/L.

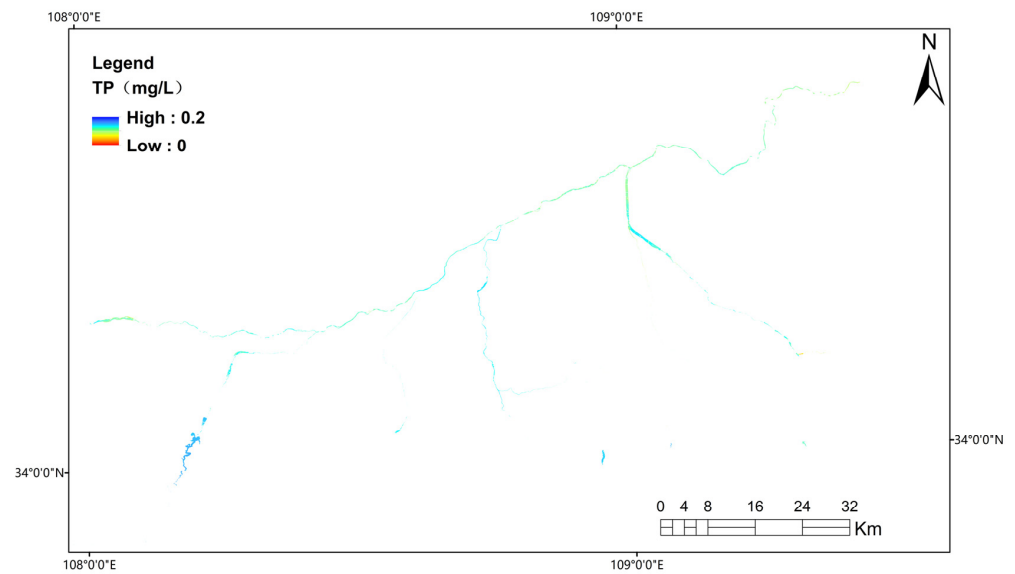


Figure 14. Distribution of TP for the Weihe River and its tributaries in December 2023 obtained from the inversion model.

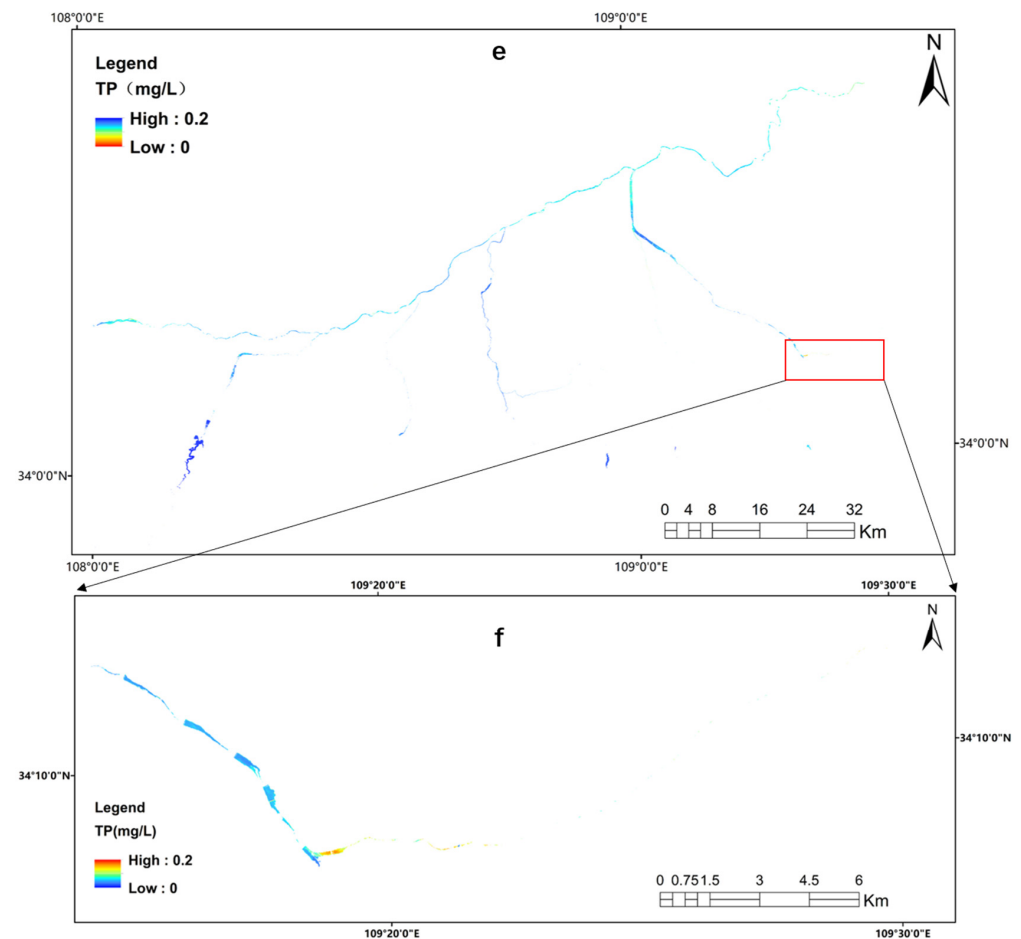


Figure 15. Distribution of TP for the Weihe River and its tributaries in December 2023 obtained from the verified model (“e” represents the overall distribution of the river, and “f” represents the river segment in the area of Lantian County).

4. Discussion

Previous studies have mostly focused on establishing inversion models for single water quality parameters. There are a few studies applying remote sensing to the modeling of the comprehensive water quality index (CWQI). The CWQI used in this study incorporates multiple water quality parameters [26,42], similar to the method used in China for defining water quality categories. Water quality categories are determined by various water parameters and their respective threshold values. If all parameters are below the concentration values for a certain level, the water body is considered to be at that level [5]. This paper establishes a simple correspondence between CWQI values and water quality categories to simplify the reference data required to determine water quality categories.

In the results of the verified model, it seems that overall, the distributions of all three parameters indicate that the water quality of the main stream of the Weihe River is generally poor, the water quality of the tributaries is better, and the water quality of the reservoir is the best. The water quality of the tributary sections near the Weihe River is worse than that of the tributary sections farther from the Weihe River. After simulating the groundwater pollution risk in the Xi'an Plain, it was found that the northern Weihe River coast of Zhouzhi County and the northern Bahe River coast of Lantian County are high-risk areas for groundwater pollution. The reason is that these areas are well-recharged by rivers, have strong aquifer permeability, and are thus easily polluted [49]. An investigation of pollution sources revealed that industrial activities are frequent in these areas, resulting in high pollution loads. This is consistent with the results of this study, as the water quality of the Bahe River near Lantian County is the lowest in the entire study area. During a study of pollution sources in the Heihe River, Jinpen Reservoir, as a key focus location, was found to have a high quality of water overall due to the absence of point source pollution upstream [50], which is consistent with the results obtained in this study.

Semi-empirical models often face limitations in temporal and spatial applicability because they typically only apply to specific temporal and spatial conditions. Different months have varying climates, and the water content and composition of river channels can differ between wet and dry seasons. For example, the water bodies extracted using NDWI are less in the dry season than in the wet season. In Ma et al.'s study [51], the research period was divided into two seasons, and the results showed significant differences in the suspended sediment concentration in the Pearl River Estuary between the dry and wet seasons. The same is true for inland water bodies, where climate change, such as evaporation and precipitation, has an impact on water quality [52].

This study established a model based on the measurement data from December 2023. The model parameters calculated from the data had small errors. After obtaining supplementary data (average values from September to November 2023), the study selected available measurement points to verify $\text{NH}_4^+\text{-N}$ and TP, and the results showed small errors (Tables 8 and 9). Additionally, the CWQI values chosen in the study can be calculated based on various parameters. However, due to the limited types of parameters available in the measurement data, this study only established a simple relationship between the measured water quality categories and the inverted CWQI values.

Table 8. Measured and verified average $\text{NH}_4^+\text{-N}$ from September to November 2023 (mg/L).

Locations	S4	S5	S7	S8	S11
Measured	0.18	0.25	0.22	0.31	0.51
Verified	0.16	0.24	0.14	0.24	0.52

Table 9. Measured and verified average TP from September to November 2023 (mg/L).

Locations	S4	S5	S7	S8	S11
Measured	0.03	0.08	0.02	0.06	0.13
Verified	0.04	0.06	0.03	0.06	0.13

In future work, we will collect a broader range of parameter data from different locations to calculate more reasonable CWQI values and establish more accurate models. Moreover, customized models will be developed for different months based on water quality parameters. This will help to further investigate the water quality changes in the Wei River and its tributaries, providing a more detailed perspective for water quality management.

5. Conclusions

In this study, we applied Sentinel-2 data (4 December 2023) to estimate the CWQI value, $\text{NH}_4^+\text{-N}$, and TP concentrations in the Weihe River and its tributaries, and analyzed the inverted and measured results. It was found that the model initially underestimated water quality. Following the regression analysis with measured data and inverted results, a verified model was obtained. The main conclusions are as follows:

The verified model shows an average relative error of only 9.80% between the estimated CWQI and measured data. The coefficients of determination (R-squared) for $\text{NH}_4^+\text{-N}$ and TP are 0.62 and 0.61, respectively. The average relative errors between estimated and measured concentrations are 19.40% and 24.70%, indicating high model accuracy in effectively reflecting the water quality status of the Weihe River and its tributaries.

The inversion results demonstrate that, following scientific management, the overall water quality of the Weihe River and its tributaries has improved. The main channel of the Weihe River shows slightly lower water quality compared to its tributaries. Tributary sections near the main channel and those near sewage treatment plants exhibit poorer water quality, with the stretch of the Bahe River between Puhua Town and Sanli Town in Lantian County being the most degraded.

The water quality issues in Lantian County warrant further investigation, which can be conducted with more comprehensive data in the future. This study can also provide an example of how to monitor water quality information using Sentinel-2 data in similar river basins.

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