Review

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Progress in Water Quality Parameter Retrieval via Remote Sensing Technique Combined with Bibliometrics

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Review

Progress in Water Quality Parameter Retrieval via Remote Sensing Technique Combined with Bibliometrics

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Abstract

Water is one of a fundamental natural resource and strategic compound. However, with socio-economic development, the water environment is being confronted with a series of problems such as aggravated pollution. Accurate monitoring of the water quality is the prerequisite and foundation for water environment supervision and governance. With the development of remote sensing and computer technologies, the retrieval of water quality parameters has attracted increasing attention from researchers and practitioners. This paper aims to present progress of remote sensing technique in water quality parameter retrieval methods and applications. The following aspects were investigated in this review: (a) water quality parameters retrieval data source; (b) water quality parameters retrieval models and evaluation metrics; (c) water quality parameters remote sensing retrieval applications; (d) some challenges and potential directions for water quality parameters retrieval. This review provides some support for researchers, as well as management departments, in theoretical research and application for remote sensing water quality parameters retrieval.

Keywords: water quality; remote sensing techniques; retrieval models; satellite data

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1. Introduction

Water resources play a crucial role in the sustainability of human and ecological systems [1–3]. Rapid urbanization and socio-economic development have caused a series of environmental issues, such as water shortages and water pollution. Effective water quality monitoring is essential for addressing the threats of water environment deterioration, as well as effective supervision and governance of the water environment [4,5].

Traditionally, water quality monitoring is based on measurements at certain sampling points, which is time-consuming, expensive, and limited to small scales. Due to the advantages of large spatial and temporal coverages, remote sensing technology makes large-scale water quality parameters retrieval possible [6–8]. Continuous, stable, and high-quality remote sensing image data are a prerequisite for remote sensing water quality parameter retrieval. Since the first civilian Earth observation satellite (Landsat) was launched in 1972, many countries have launched satellite systems, which provide various and stable remote sensing images and water environment monitoring services [9–13]. In recent years, aerial remote sensing data, as well as ground data, have also provided rich data sources for water quality parameters retrieval [14–16].

Based on rich remote sensing data sources, scholars have explored various water quality parameter retrieval models and algorithms in the past few decades. Bibliometric analysis shows that the number of research publications has increased each year [17–19]. The water quality parameter retrieval models mainly include bio-optical, empirical, semi-empirical and artificial intelligence models (AI) [20–23]. The bio-optical models take into account the retrieval mechanism of water quality parameters with a higher accuracy. Empirical models establish mathematical relationships between water quality parameters and reflectance to obtain water quality parameters. Semi-empirical models consider the mechanism and spectral characteristics of water quality parameters. Compared with traditional empirical and semi-empirical models, AI models have unique advantages in explaining these complex relationships, as well as in achieving a higher accuracy.

The key to water quality parameters retrieval by remote sensing technique is to establish relationships between water quality parameters and the reflection of water bodies. Due to the distinct spectral characteristics, most research and applications have focused on three major components, namely, chlorophyll-a (Chl-a), total suspended solids (TSS), and colored dissolved organic matter (CDOM)[24,25] in early water quality remote sensing research. With the improvement of the spectral resolutions of sensors, some water quality parameters without obvious spectral response characteristics, such as the total nitrogen (TN), total phosphorus (TP), ammonia nitrogen (NH_3N), dissolved oxygen (DO), and chemical oxygen demand (COD), are increasingly being retrieved [26–29].

In the past few decades, remote sensing technology has achieved great success in water quality parameter retrieval, with a series of high-precision and stable models aiding in water quality parameters retrieval. To demonstrate the advancements in the use of remote sensing for water quality parameters retrieval, this paper reviews the latest progress in quantitative water quality estimation in terms of the research trends, data sources, retrieval models, and several water quality parameters retrieval applications. Furthermore, the current challenges and possible solutions are discussed.

2. Bibliometric Analysis

The Web of Science (WOS) and CiteSpace were chosen as the analysis tools for the bibliometric analysis. According to the statement of "TI=(("water quality parameter" OR "water quality" OR "water parameter")NOT("land*")NOT("vegeta*") NOT("drink*")NOT("sea")) " and TS=("RS" OR "remote sens*" OR "remotely sens*" OR "spectr*"), the irrelevant literature was removed, and 1311 papers were obtained for subsequent analysis.

The trend of the number of water quality papers published during the period 2000–2024 is shown in Figure 1. The bar chart suggests that the publication volume of water quality papers has been increasing since 2000. To reflect the changes in the proportion of water quality literature to remote sensing literature, the proportion of water quality to remote sensing is also presented. The results indicate that water quality has attracted increasing attention in remote sensing research.

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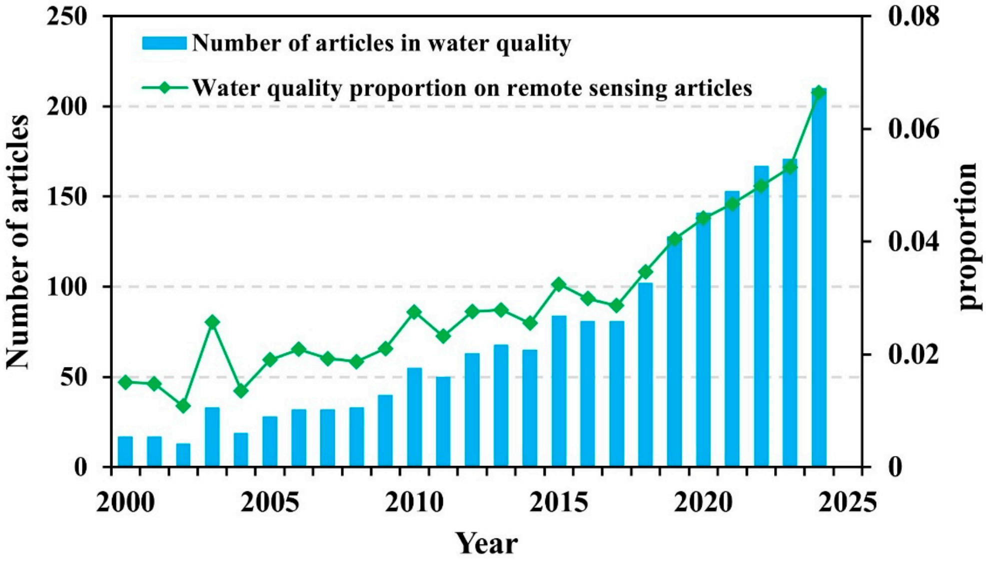

Figure 1. Number of published articles on water quality and its proportion to remote sensing literature.

Figure 2 shows a pie chart of the proportion of published papers in the top 10 countries. The top 10 countries account for approximately 90% of the total publication of water quality remote sensing literature, forming the main pillars in this direction. More specifically, China has made significant contributions in this field, accounting for over 40% of all publications, followed by the United States (approximately 20%).

According to the publications of water quality remote sensing articles, a statistical table of the number of articles in publications indexed by the WOS was created (Table 1). In terms of publications, *Remote Sensing* accounts for the largest proportion (approximately 18%), followed by *The Science of the Total Environment* and *Water* (16.1% and 11.4%, respectively).

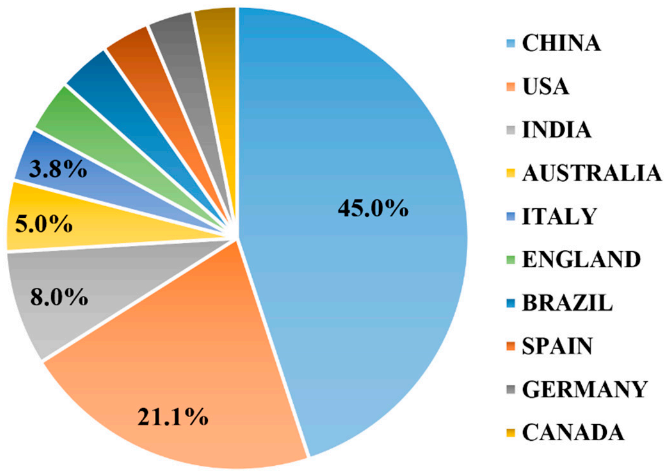

Figure 2. Proportion of articles published by top 10 countries.

Table 1. Statistics on the number of publications indexed by the WOS.

Ranking	Publication	Record Count
1	REMOTE SENSING	102
2	THE SCIENCE OF THE TOTAL ENVIRONMENT	89
3	WATER	63
4	ENVIRONMENTAL MONITORING AND ASSESSMENT	50

5	IEEE INTERNATIONAL SYMPOSIUM ON GEOSCIENCE AND REMOTE SENSING IGARSS	49
6	PROCEEDINGS OF SPIE	45
7	ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH	41
8	ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH INTERNATIONAL	41
9	SPECTROSCOPY AND SPECTRAL ANALYSIS	41
10	PROCEEDINGS OF THE SPIE THE INTERNATIONAL SOCIETY FOR OPTICAL ENGINEERING	32

Figure 3 shows the keywords appearing in the collected articles from 2000 to 2024. An annual analysis of the keywords in the bibliographic data was conducted, and a co-citation analysis of the keywords was performed using CiteSpace. The time scale was from 2000 to 2024, the time slice was set to 1, and the node type was set to keywords. Labels were assigned based on the frequency of occurrence. The visualization graph shows that Chl-a, DO, TP, and TN were the main water quality parameters studied; rivers, lakes, and coastal zones were the main research areas; and machine learning and deep learning were the research methods commonly used.

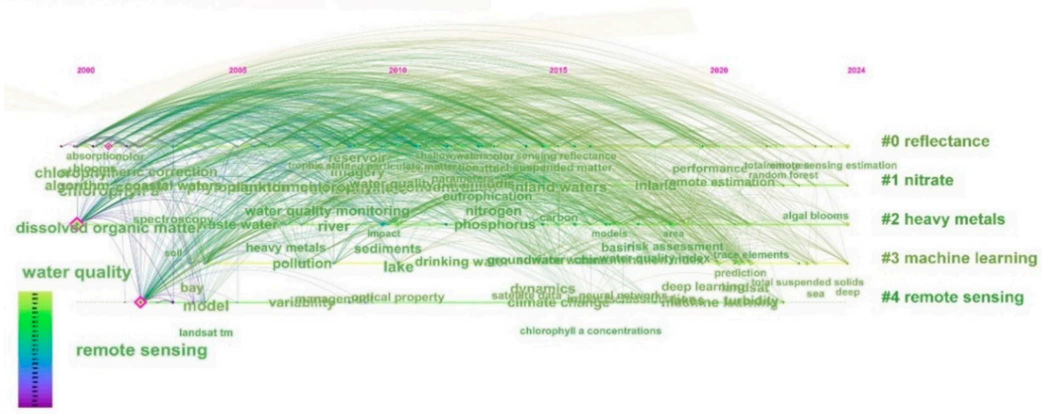

Figure 3. Visualization of the keyword network for the period 2000–2024.

3. Water Quality Parameters Retrieval Data Acquisition

The radiation information about water surfaces at various wavelengths can be recorded by remote sensors, which include satellite, aviation, ground, airship data. This section mainly introduces satellite, aviation and ground data.

3.1. Satellite Data

With the development of remote sensing technology and the increasing demand for applications, the United States, Europe, China, Russia, Japan, Canada, India, and other countries and regions have operated several satellite systems to provide considerable remote sensing images and Earth observation services in the past few decades. According to the spatial resolution, satellite remote sensing images can be divided into coarse-, medium-, and high-spatial-resolution images, the parameters of which are presented in Table 2.

The coarse-spatial-resolution satellites for water quality parameters retrieval mainly include the Advanced Very High Resolution Radiometer (AVHRR) onboard the National Oceanic and Atmospheric Administration (NOAA) satellites, Moderate Resolution Imaging Spectroradiometer (MODIS), Medium Resolution Imaging Spectrometer (MERIS), Geostationary Ocean Color Imager (GOCI), and Sentinel-3 Ocean and Land Color Instrument (OLCI)[30–33]. Due to the short revisit period and high signal-to-noise ratio, the coarse-spatial-resolution satellite data have significant advantages in large-scale and even global-scale water environment research.

Common medium-resolution remote sensing sensors mainly include the Landsat multi-spectral scanner (MSS)/thematic mapper (TM)/enhanced thematic mapper plus (ETM+)/operational land imager (OLI), SPOT 1–4, Hyperion, and Sentinel-2 Multi-spectral Instrument (MSI)[34–37]. Because of the good agreement of their temporal, spatial, and spectral resolutions, the medium-resolution optical images have large advantages in regional water quality parameters retrieval, while they have limitations in terms of instantaneous changes in retrieval results under cloudy and rainy weather.

The high-spatial-resolution remote sensing used in water quality parameters retrieval mainly include IKONOS, QuickBird, WorldView, SPOT series. It is worth noting that China has launched a series of high-resolution remote sensing satellites, including the Gaofen (GF), Zhuhai, Ziyuan (ZY) and Beijing series satellites in recent years. These high-spatial-resolution satellites have effectively promoted the application of water environment monitoring, especially in urban areas[38–40].

Table 2. Technical specifications of common satellite remote sensors used in water quality parameters retrieval.

Category	Sensor	Height on orbit (km)	Orbital swath (km)	Spatial resolution (m)	Temporal resolution (day)	Bands	Spectral range (nm)
Coarse resolution	AVHRR	833–870	2800	1100	0.5	5	550–12,500
	MODIS	705	2330	250–1000	0.5	36	400–14,400
	GOCI	35,837	2500	500	1/24	8	402–885
	MERIS	790 ± 10	1150	300	3	22	465–2135
	Sentinel-3	814.5	1270	300	2	21	400–1020
Medium resolution	Landsat 1–3	907–915	185	78	18	4	500–1100
	Landsat-4/5	705	185	30–120	16	7	450–12,500
	Landsat-7	705	185	15–60	16	8	450–12,500
	Landsat-8	705	185	15–100	16	11	430–12,510
	Landsat-9	705	185	15–100	16	11	435–12,500
	SPOT 1–4	822	60	10–20	26	4–5	500–1750
	Hyperion	705	7.7	30	200	242	400–2500
	Sentinel-2	786	290	10–60	5	13	420–2300
High resolution	IKONOS	681	11.3	0.82–4	1.5–3	5	445–900
	QuickBird	450–482	16.8–18	0.61–2.88	1–6	5	450–900
	WorldView 1–4	496	17.6	0.31–3.7	1.7–5.9	4–28	450–800
	SPOT 5	822	60	2.5–20	26	5	480–1750
	SPOT 6/7	694	60	1.5–6	26	5	500–890
	ZY-3	506	50	2.1–5.8	3–5	7	500–890
	GF-1/2/6	631–645	45–90	0.8–16	1–5	5–13	450–900
	Zhuhai-1	500	150	0.44–10	1–32	32	400–1000
	Beijing-3	500-700	12	0.3–0.5 1.2–2	— —	4–6	400–900

3.2. Aviation Data

With the miniaturization of hardware equipment, multispectral and hyperspectral remote sensing data based on human-machine and unmanned aerial vehicle (UAV) platforms have begun to be applied in the field of water quality parameters retrieval [41–43]. Compared with satellite platform, the flight time, heights and route of the aircraft platform can be selected according to the actual demand. Image data obtained by aircraft platform with a higher spatial resolution, which can reflect the spectral and spatial information about water bodies better, thus improving the accuracy of water quality parameters retrieval [44–47].

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The commonly used manned airborne systems include HyMAP-C developed in Australia, the Prob series developed in the United States, CASI/SASI/TASI developed in Canada, AISA+ developed in Finland, and PHI developed in China. Current UAV platform-based hyperspectral equipment mainly includes OCI developed in the United States, SPECIM developed in Finland, HySpex developed in Norway, and small imaging hyperspectral systems developed by the Changchun Institute of Optics, Fine Mechanics and Physics, the Shanghai Institute of Technical Physics, and Aerospace Information Research Institute, Chinese Academy of Sciences. Table 3 lists the technical specifications of common airborne hyperspectral remote sensors.

Table 3. Technical specifications of common airborne remote sensors used in water quality parameters retrieval.

Sensors	Spectral range (nm)	Number of channels	Spectral resolution (nm)	Field of view (°)	Imaging mode
AVIRIS	380–2500	224	10	34	Spectroscopic, scanning
CASI-1500	380–1050	Adjustable, up to 288	<3.5	40	Spectroscopic, push-broom
PHI	400–850	244	<5	21	Spectroscopic, push-broom
OMIS-II	400–1100	64	10	>70	Spectroscopic, scanning
HyMap	400–2500	128	15–20	60	Spectroscopic, scanning
AISA	430–900	288	3	38	Spectroscopic, scanning

3.3. Ground Data

Field spectrometers can flexibly and inexpensively obtain spectral data on ground objects, which is widely used for water spectral data acquisition[48–50]. Currently, the main manufacturers of field spectrometers include Ocean Optics (US), ASD (US), and Avantes (Netherlands). Ground spectrometers commonly used in water spectra data acquisition include the FieldSpec 4, USB4000, and Torus series miniature spectrometers. Although micro spectrometers cannot compare with large spectrometers in resolution and spectral range, they have the advantages of portability, intelligence, and integrations. The technical specifications of common ground field spectrometers are presented in Table 4.

Table 4. Technical specifications of common ground field spectrometers used in water quality parameters retrieval.

Manufacturer	Spectrometer	Spectral range (nm)	Number of channels	Spectral resolution (nm)
Spectral Evolution	PSR-3500	350–2500	1024	3.5 (350–1000 nm) 10 (1000–1500 nm) 7 (1500–2100 nm)
SVC	SVC 1024	350–2500	1024	3.5 (350–1000 nm) 9.5 (1000–1900 nm)
ASD	FieldSpec 4	350–2500	2151	3 (350–1000 nm) 8 (1000–2500 nm)
Ocean Optics	USB-4000	200–1100	Configuration dependent	0.1–10

4. Water Quality Parameters Retrieval Models and Evaluation

4.1. Bio-Optical Model

The bio-optical model is based on radiation transmission models. The upstream and downstream irradiance of the water body is calculated, and then, the relationship between the upstream and downstream irradiance, absorption coefficient, and backscattering coefficient of each component of the water body is established[51–53]. The principle of the bio-optical model is shown in the equation (1):

$$R(0,\lambda) = f\frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \tag{1}$$

where $R(0,\lambda)$ is the ratio of the upward irradiance to downward irradiance on the surface of the water body at wavelength λ, $a(\lambda)$ is the absorption coefficient of the water body, $b_b(\lambda)$ is the backscattering coefficient of the water body, and f is a variable parameter. $a(\lambda)$ and $b_b(\lambda)$ are the linear sums of the contributions of each component of the water body.

The bio-optical model has a clear theoretical basis and physical significance, and it depends less on the measured sample points, which makes it easy to analyze sources of error with higher universality[54,55]. However, the composition of the water body and radiation transmission procedure are rather complex, and many input parameters (such as inherent optical characteristics, surface tourism characteristics, and water quality variables) still need to be measured, which limits practical applications. Some examples of water quality parameters studied using bio-optical models are presented in Table 5.

Table 5. Some studies of water quality parameter retrieval using optical models.

Model	Water parameters	References
2SeaColor	Chl-a, TSS, CDOM	[56]
QAA	Chl-a	[57]
LM	CDOM	[58]
GSM	Chl-a	[59]

4.2. Empirical Models

Empirical models were developed in early applications for water quality parameter retrieval using multispectral remote sensing data. In these models, the correlations between the remote sensing reflectance and water quality parameter values are calculated, and then, the optimal band or band combination is selected. Finally, the water quality parameter values of unmeasured points are calculated through the statistical relationships established[60–64].

The advantages of empirical models are that the relationships between the remote sensing reflectance and water quality parameters are easy to establish and that the model is simple and feasible. The disadvantage is that the explanation of the model mechanism is insufficient, resulting in poor applicability of the model. It is also easily limited by the research area and data. Empirical models mainly include the single band method, logarithmic method, spectral differentiation method, ratio method, and difference method[65,66]. The calculation equations are presented in Table 6.

Table 6. Common empirical models for water quality parameter retrieval.

Model	Equation	Reference
Single band	$C_{water} = a \times R_\lambda + b$	[67]
Logarithmic	$C_{water} = a \times \log{(R_\lambda)} + b$	[68]
Spectral Differentiation	$C_{water} = a \times (R_{\lambda_i})^n + b$, $R_{\lambda_i} = \frac{(R_{\lambda_{i+1}})^n - (R_{\lambda_{i-1}})^n}{\lambda_{i+1} - \lambda_{i-1}}$	[69]

Ratio	$C_{water} = a \times \frac{R_{\lambda 1}}{R_{\lambda 2}} + b$	[70]
Difference	$C_{water} = a \times (R_{\lambda 1} - R_{\lambda 2}) + b$	[71]

Note: R_λ is the remote sensing reflectance of water at wavelength λ, and a and b are regression coefficients.

4.3. Semi-Empirical Models

Semi-empirical models were developed for the application of hyperspectral remote sensing in water quality parameters retrieval. Based on the empirical model, the semi-empirical model considers the spectral characteristics and other prior knowledge of water quality parameter retrieval[72–74]. Then, the optimal band or band combination is selected, and the relationships between remote sensing reflectance and water quality parameters are established using appropriate mathematical methods.

Semi-empirical models partially make up for the defects of empirical models in water quality parameter retrieval, while they are limited to a special time and region because they depend on synchronization of the measured water quality data and remote sensing observation data[66,75]. Semi-empirical models commonly used for water quality parameter retrieval include the three-band method, four-band method, APPLE model, and Tassan model, whose calculation equations are presented in Table 7.

Table 7. Common semi-empirical models for water quality parameter retrieval.

Model	Equation	Water parameter	Reference
Three-band	$C_{water} = a \times ((R_{\lambda 1})^{-1} - (R_{\lambda 2})^{-1}) \times R_{\lambda 3} + b$	Chl-a	[76]
Four-band	$C_{water} = a \times \frac{(R_{\lambda 1})^{-1} - (R_{\lambda 2})^{-1}}{(R_{\lambda 3})^{-1} - (R_{\lambda 4})^{-1}} + b$	Chl-a	[77]
APPLE	$C_{water} = a \times F(APPLE) + b$ $F(APPLE) = R_{NIR} - [(R_{BLUE} - R_{NIR}) \times R_{NIR} + (R_{RED} - R_{NIR})]$	Chl-a	[78]
Tassan	$C_{water} = a \times \frac{R_{\lambda 1} + R_{\lambda 2}}{R_{\lambda 3}/R_{\lambda 4}} + b$	TSS	[79]

Note: $R_{\lambda 1}, R_{\lambda 2}, R_{\lambda 3}$, and $R_{\lambda 4}$ are the remote sensing reflectance of the water body at wavelengths $\lambda 1$, $\lambda 2$, $\lambda 3$, and $\lambda 4$, respectively; and a and b are the regression coefficients.

4.4. Artificial Intelligence Model

4.4.1. Machine Learning Model

As a branch of computer science, machine learning models have been widely applied in water quality parameter retrieval due to its good computational performances and nonlinear mapping abilities[80,81]. Many researchers have analyzed the relationships between water quality parameters and the spectral reflectance based on measured data[82–84]. The influence mechanism of spectral characteristics of various elements in water bodies is unclear, while machine learning models has certain advantages in solving these complex problems because of its black box mode, as well as in effectively improving the accuracy of water quality parameter retrieval.

The machine learning water quality parameters retrieval models commonly used mainly include support vector regression (SVR), random forest (RF), extreme gradient boosting (XGBoost), adaptive boosting (Adaboost), multilayer perceptron (MLP), backpropagation network (BP)[85–87]. Similar to empirical and semi-empirical models, the accuracy of machine learning models is also greatly affected by the study area and sample point distribution. Some studies on water quality parameter retrieval using machine learning models are listed in Table 8.

Table 8. Some studies on water quality parameter retrieval using machine learning models.

Study area	Data source	Method	Water parameter	Reference
Valle de Bravo reservoir	MERIS	LR, RF, SVR, GPR	Turbidity	[88]
Nandu River	Landsat 8	SVR, RF, ANN, RT, GBM	TN, TP, NH_3N	[89]
Beigong Reservoir	UAV hyperspectral image	Adaboost, Gradient Boost, SVR, RF	Chl-a, TSS	[90]
Zhanghe River	UAV multispectral image	BP, RF, XGBoost	Chl-a, TP, TN, COD_{Mn}	[91]
Yuhe river	Near-surface hyperspectral spectra	LASSO, DTR, SVR, MLP	COD, NH_3N, DO	[92]
Yangtze River	Sentinel-2, Landsat-8, GF-1	GA-RF	TP, TN	[93]

4.4.2. Deep Learning Model

With the development of computer technology and the improvement of the performance of computer hardware equipment, deep learning models have been shown to have great superiority in remote sensing image classification and spectral information reconstruction, which provide new technical methods for water quality parameters retrieval. Traditional regression methods have difficulty extracting deep spectral information from spectral data. There are multiple hidden layers between the input and output layers of deep learning models, which can effectively simulate complex nonlinear relationships between spectral and water quality parameters data so as to achieve a higher accuracy in water quality parameter retrieval and better revealing the spatiotemporal distribution patterns of water quality parameters [94–97]. However, deep learning models also have problems such as unclear mechanisms and low model universality. Some examples of the use of deep learning models to invert water quality parameters are presented in Table 9.

Table 9. Some studies on water quality parameter retrieval using deep learning models.

Study area	Data source	Model	Water quality	Reference
Maozhou River	UAV hyperspectral image	HF-DFM	Chl-a, COD	[98]
Guanhe River	Airborne hyperspectral image	DNNR	TP, TN, COD, NH_3N	[99]
Simcoe Lake	Landsat	MDL	Chl-a, TP, TN	[100]
Balik Lake	Sentinel-2	CNN	Chl-a	[101]
Liangzi lake	Sentinel-2	DNN	Chl-a，TSS	[102]

4.5. Model Evaluation Metrics

Appropriate evaluation metrics can be used to assess the accuracy of model training, over-fitting or under-fitting correction, and model transferability. Based on the research status and progress, the following model evaluation metrics are summarized: the coefficient of determination (R^2), root mean square error (RMSE), mean square error (MSE), mean absolute error (MAE), relative error (RE), and residual prediction deviation (RPD). The equations of these metrics are as equation (2) to (7):

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - y_i')^2}{\sum_{i=1}^{n}(y_i' - \bar{y})^2} \tag{2}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - y_i')^2} \tag{3}$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - y_i')^2 \tag{4}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - y_i'| \tag{5}$$

$$RE = 100 \times \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i - y_i'|}{y_i} \tag{6}$$

$$RPD = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - y_i')^2}} \tag{7}$$

where y is the average value, and y_i and y_i' are the observed and predicted values of observation point i, respectively. Among these metrics, R^2 is the most commonly used and accepted evaluation metric. Excessive pursuit of a higher R^2 value may lead to over-fitting and poor transferability of the model. Therefore, R^2 is usually used in combination with other evaluation metrics to balance the fitting accuracy, portability, and computational complexity of the model, as well as enabling a more objective and comprehensive evaluation of the model.

5. Water Quality Parameter Retrieval Via Remote Sensing Techniques

5.1. Chlorophyll-a

Chl-a is the most basic indicator of the trophic state of water bodies, which can indicate the distribution of plankton biomass[103,104]. The spectral characteristics of chlorophyll include strong absorption between 450 and 475 nm and at 670 nm, and peaks at 550 nm and near 700 nm[105,106]. The reflection peak at 700 nm is a typical spectral feature of chlorophyll-a, which is of great significance for estimating chlorophyll in water bodies. The peak position of water spectra shifts from approximately 680 nm to 710 nm as the peak amplitude value increases due to an increase in the Chl-a concentration.

Table 10. Some studies on Chl-a retrieval.

Study area	Data source	Model	R²	Reference
A lake in North Carolina, USA	Sentinel-2	XGBoost, random forest,	0.64	[107]
Chaohu Lake, China	GF-1	Normalized difference chlorophyll index	0.93	[108]
Pearl River Estuary, China	Landsat 5/7	Two-band global algorithm	0.71	[109]
Poyang Lake, China	GF-1	APPEL model	greater than 0.6	[110]
Nanpaishui River, Nanyun River	UAV multispectral and hyperspectral imagery	stepwise regression	0.77	[111]
Hedi reservoir, Gaozhou reservoir	Sentinel-2	GA–ANN	0.87	[112]

In addition to the optical properties of phytoplankton, the optical properties of inland and coastal water bodies are determined by a composite of dissolved organic matter, dead particles, organic matter, and inorganic particles from land-based sources[113–116]. Therefore, retrieval of the Chl-a concentration is much more complex and less accurate, and as a result, these components are not statistically correlated. Based on the absorption and reflection characteristics, a series of algorithms have been developed to retrieve the Chl-a concentration. Several models for retrieving the Chl-a concentration are listed in Table 10.

5.2. Total Suspended Solids

The TSS concentration is one of the key water quality parameters for water bodies. It is related to incoming sunlight, which affects photosynthesis for the growth of algae and plankton, as well as the primary productivity of the water body. The TSS have reflectance spectral characteristics at 580–680 nm and 700–900 nm. Many studies have shown that when chosen appropriately, a single band or a combination of bands can achieve a high accuracy in TSS retrieval[117,118]. However, the reflectance of water is affected by the complex substances in the water body, so different spectral bands can be used for TSS retrieval. Some models for retrieving the TSS concentration are summarized in Table 11.

Table 11. Some studies on TSS retrieval.

Study area	Data source	Model	R^2	Reference
Lake Chapala	Landsat 5-8	Multiple linear regression	0.81	[119]
A lake at South Brazil	Landsat 8	Artificial Neural Network	0.6	[120]
Poyang Lake	Sentinel-2	Exponential model	0.93	[121]
Yangtze River	MODIS	Ratio model	0.88	[122]
Deep Bay, China	MODIS	Exponential retrieval model	0.62	[123]

5.3. Total Phosphorus and Total Nitrogen

The TP and TN in water bodies mainly come from the external environment and the release of the water itself[124,125]. Excessive nitrogen and phosphorus concentrations can lead to microbial proliferation, the rapid growth of plankton, and eutrophication of water bodies, resulting in further deterioration of the water quality. Scientific and accurate retrieval of nitrogen and phosphorus is the premise and foundation for controlling nitrogen and phosphorus source pollution.

Currently, research on water quality parameters retrieval through remote sensing has mainly focused on the three major components, including the concentrations of chlorophyll, TSS and CDOM. Numerous scholars have conducted studies on TP and TN retrieval by remote sensing, while the TP and TN concentrations, as optically insensitive water quality parameters, are theoretically difficult to invert using physical models, which poses significant challenges[126–129]. The currently used methods for TP and TN retrieval can be mainly divided into direct and indirect methods.

5.3.1. Direct Methods

The direct methods establish a retrieval model for the TP and TN concentrations by calculating the relationships between the remote sensing reflectance (Rrs) and the measured water quality parameters. The direct methods estimate the TP and TN concentrations using statistical methods. However, the direct methods fail to consider the underlying mechanisms of TP and TN, and the retrieval results are largely dependent on the study and measured data, leading to limited applicability. Relevant studies on the retrieval of the TP and TN concentrations using direct methods are listed in Table 12.

Table 12. Some studies on TP and TN retrieval using direct models.

Study area	Data source	Water quality	References
Balik Lake	MODIS	TP, TN	[130]
Burullus Lake	Sentinel-2	TP, TN	[131]
Poyang Lake, Dongting Lake, Taihu Lake	Landsat 8	TP, TN	[132]
Taihu Lake	proximal hyperspectral imager	TP, TN	[133]
Taihu Lake	MODIS	TP	[134]
Pearl River Estuary	Landsat 8	TP, TN	[135]
Dongping Lake	Landsat 8	TP, TN	[136]
Yellow River Delta	Sentinel-2	TP, TN	[137]

5.3.2. Indirect Methods

Chl-a, TSS, and CDOM have well-defined optical properties and spectral responses. Many studies have shown that there is a correlation between the chlorophyll, TP, and TN concentrations, which provides a theoretical basis for TP and TN retrieval using chlorophyll-sensitive wavelengths[138–142]. The TP and TN concentrations are related to the concentrations of optically active water quality parameters, which can be determined using the equation (8):

$$(TP, TN) \propto f(Chl - a, TSS, CDOM) \tag{8}$$

That is, the concentrations of TP and TN are positively correlated with the Chl-a, TSS, and CDOM concentrations and other water quality parameters, and the concentrations of these parameters can be obtained by remote sensing methods.

$$f(Chl - a, TSS, CDOM) \propto R_{rs} \tag{9}$$

Based on equations (8) and (9), the relationship between the TP and TN concentrations of the water and the remote sensing reflectance is as following equation (10):

$$(TP, TN) \propto R_{rs}. \tag{10}$$

The indirect methods establish the relationship between the TP and TN concentrations and optically active water quality parameters, and then, the TP and TN concentrations are calculated indirectly according to the retrieval results of the optically active water quality parameters[143]. Compared with the direct methods, the indirect methods consider the remote sensing retrieval mechanism of the TP and TN concentrations. The retrieval results of the optically active water quality parameters, as well as the correlation between the optically active water quality parameters, affect the accuracy of the retrieval results of TP and TN.

6. Challenges and Future Development

1. Water Quality Parameters Retrieval of Small-scale River and Lakes

Currently, most satellite data are mainly suitable for large-scale water quality parameters retrieval. There are several challenges in water quality parameters retrieval of small lakes and narrow rivers in urban areas because of the limitations in fine spectral, spatial, and temporal resolutions of remote sensing data. Therefore, future research could focus on integrate satellite, aviation, and ground data to meet the needs of long-term and fine-scale regional studies. Meanwhile, regional high-spatiotemporal-resolution data can be obtained through autonomously operate and control satellites along any trajectory, or through data fusion methods.

2. Interpretable Deep Learning Water Quality Parameter Retrieval Models

Although machine learning models have the significant advantage of the occurrence of nonlinear relationships between the water reflectance and water quality parameters, there are still some challenges. First, a single machine learning model has some shortcomings such as over-fitting, high dimensionality, and slow convergence. Second, data-driven methods, represented by empirical and machine learning methods, have difficulty explaining physical mechanisms, which limits the accuracies and generalization abilities of these models. The attainment of a large amount of measured data and the use of integrated machine learning are notable research directions. In addition, model optimization and improvement should be combined with inherent optical properties to enrich the physical significance of data-driven methods.

3. Water Quality Parameter Retrieval Models Integrating Multiple Environmental Factors

Most previous studies focused on three major components of the ocean color, namely the Chl-a, CDOM, and TSS concentrations, while additional parameters (including TP, TN, NH_3-N, DO concentrations, and COD) are not well investigated because of the weak optical characteristics. Given the complexity of the water environment, revised water quality models are generally established for certain regional water bodies, to retrieval water quality parameters more accurately. In future research, the influences of various environmental factors should be considered to retrieval multiple water quality parameters.

7. Conclusions

Good water quality is crucial for human survival and health, ecological balance, and sustainable socio-economic development. Over the past few decades, numerous scholars have developed a series of algorithms for remote sensing water quality parameter retrieval based on multi-platform remote sensing data. This review provides a comprehensive introduction to remote sensing water quality parameter retrieval, including literature analysis, remote sensing data sources, retrieval models, several water quality parameter retrieval application, current challenges, and future development directions.

From 2000 to 2024, the number of published papers on water quality remote sensing increased each year. The research hotspots mainly included remote sensing, Chl-a, DO, TP, and TN. A series of satellite, aviation, and ground data were used for remote sensing water quality parameter retrieval. In terms of the spatial resolution, remote sensing data can be divided into high-, medium-, and low-resolution data. Water quality parameter retrieval models include bio-optical, empirical, semi-empirical, and AI models. Several water quality parameters (such as Chl-a, TSS, TP, and TN) have been extensively studied. Among them, Chl-a and TSS have distinct spectral characteristics, thus can be retrieved by empirical or semi-empirical models. However, the optical characteristics of TP and TN are unclear, usually retrieved using both direct and indirect methods. Future research could establish interpretable deep learning models considering multiple environmental factors to retrieval water quality parameters more accurately. At the same time, water quality parameters retrieval of small-scale river and lakes should also be paid more attention.

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Abbreviations

Adaboost	adaptive boosting
BP	backpropagation network
CDOM	colored dissolved organic matter
Chl-a	chlorophyll-a
COD	chemical oxygen demand
DO	dissolved oxygen
MAE	mean absolute error
ML	machine learning
MLP	multilayer perceptron
MSE	mean square error
R^2	coefficient of determination
RE	relative error
RF	random forest
RMSE	root mean square error
RPD	residual prediction deviation
Rrs	remote sensing reflectance
SVR	support vector regression
TN	total nitrogen
TP	total phosphorus
TSS	total suspended solids
UAV	unmanned aerial vehicle
WOS	Web of Science
XGBoost	extreme gradient boosting

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