RESEARCH PAPER

Integrated Surface Water Quality Assessment and Prediction for Sustainable Water Resource Management

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Abstract

Surface water represents one of the most critical freshwater resources supporting domestic, agricultural, industrial, ecological, and socioeconomic development worldwide. However, rapid urbanization, industrialization, agricultural intensification, population growth, and unregulated anthropogenic activities have resulted in severe deterioration of surface water quality across many developing regions. The increasing occurrence of elevated dissolved salts, excessive hardness, toxic heavy metals, microbial contamination, and other physicochemical pollutants has become a major environmental and public health concern, emphasizing the urgent need for comprehensive water quality assessment and sustainable management strategies. Conventional monitoring approaches effectively characterize present water quality conditions but provide limited capability for predicting future deterioration and supporting long-term environmental planning.

Keywords: Surface Water Quality; Surface Water Assessment; Environmental Monitoring; Water Resource Management; Sustainable Development.

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Introduction

Surface water is an important resource for domestic supply, agriculture, industry, ecosystem functioning and socio-economic development, and an integral part of the global hydrological cycle. Rivers, lakes, reservoirs and streams provide water for human activities and at the same time support aquatic habitats, nutrient cycling and ecological processes. Increasing demand for fresh water driven by population growth, urbanization and economic development has put more pressure on available surface water resources. Thus, the adequate water quality has become a key element of environmental sustainability, public health protection and integrated water resources management. The quality of surface water is influenced by natural processes and anthropogenic activities. Chemical characteristics of water are influenced by natural processes such as weathering of rocks, mineral dissolution, erosion, sediment transport and climatic variability. However, the pace of urbanization and industrialization has increased the anthropogenic pressure on river systems manifold. Various contaminants can be introduced into surface-water bodies by domestic wastewater, industrial effluents, agricultural runoff, solid-waste disposal, construction activities and uncontrolled drainage. These inputs can alter the physical, chemical and biological characteristics of water and can gradually decrease its suitability for domestic, agricultural, industrial and ecological uses.

Physicochemical characteristics provide basic information on the state of surface-water resources. The general chemical condition of water is usually described by parameters like pH, total dissolved solids (TDS), electrical conductivity, hardness, chloride, sulfate, turbidity, color and major ions. High dissolved solids and ionic constituents can be indicative of mineralization, saline intrusion, wastewater inputs, or other anthropogenic influences; excessive hardness can be problematic for domestic and industrial uses. Increased turbidity and color may be indicative of suspended sediments, organic matter, wastewater discharges and surface run-off. Hence, systematic evaluation of physicochemical parameters is required to detect the major changes in water quality and to ascertain the potential suitability of surface water for specific uses. Besides physicochemical degradation, contamination by potentially toxic metals is a major environmental concern. Metals such as lead, cadmium, chromium, iron, manganese and aluminum may be introduced to surface waters from industrial discharges, urban runoff, mining activities, corrosion, atmospheric deposition and natural geological processes. Certain metals, unlike many biodegradable organic contaminants, may persist in aquatic environments and may accumulate in sediments and biological organisms. Prolonged exposure to high concentrations of toxic metals can have detrimental effects on aquatic ecosystems and human health. Therefore, heavy-metal assessment is an important component of comprehensive surface-water-quality monitoring. Microbiological contamination is another important aspect of surface-water quality. Domestic wastewater, sewage, animal waste and contaminated runoff that enter rivers may contain indicator organisms, which are evidence of microbiological pollution. Total coliforms are often used as general indicators of water microbial quality, while Escherichia coli is generally considered a more specific indicator of fecal contamination. The presence of microbial indicators is especially important when surface water is considered for domestic or potable applications as untreated contaminated water may pose potential public-health risks. Therefore, microbiological parameters should be evaluated in conjunction with physicochemical and chemical parameters not in isolation. Organic contaminants, including pesticides, petroleum hydrocarbons, polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), and other persistent organic pollutants, can also contribute to the degradation of surface water. Their presence is related to adjacent land use, agricultural and industrial activities, wastewater inputs and contaminant transport pathways. Such contaminants may be present in trace concentrations but some persistent compounds can persist in the environment for long periods and can be bioaccumulated or biomagnified. Therefore, the screening of selected organic pollutants may provide additional evidence concerning the nature and sources of surface-water contamination. The traditional approach to surface-water quality assessment has been to resort to field sampling, laboratory analysis and comparison with established water-quality standards or guideline values . These approaches are still essential if one is to obtain reliable information on the present status of water resources. The conventional monitoring is, however, often limited by the number of sampling locations, sampling frequency, seasonal variability, laboratory costs and availability of long-term datasets. A limited number of samples may be sufficient to describe water quality at a particular location and time, but may not fully represent the spatial and temporal variability of contamination. Hence, the integration of multiple water-quality parameters and interpretation of their combined effects becomes increasingly important for effective environmental assessment. Therefore a full assessment of surface-water quality should take into account the combined effect of physicochemical, chemical, microbiological and organic contaminants. The assessment based on one single parameter may give an incomplete picture of the water-quality status as different contamination processes may occur simultaneously. For example, increased dissolved solids may be due to mineral or wastewater derived inputs, while concurrent increases in turbidity, heavy metals and microbial indicators may indicate additional anthropogenic pressures. An integrated assessment can thus offer a more reliable basis for identifying the critical water quality problems and deciding on the necessary management and treatment requirements. Interpretation of surface-water quality also depends on the intended use of the water resource. Water that is acceptable for some ecological or recreational uses may not be acceptable for domestic or potable use. Thus, in the assessment of surface water suitability it is required to compare with relevant national and international water quality criteria. This type of comparison can help identify parameters that are above recommended limits and prioritize contaminants for treatment or management intervention. Understanding the relative importance and spatial distribution of these contaminant groups is critical to designing appropriate treatment strategies and to establishing effective water resource management practices.

2. Literature Review

Surface water is one of the most important freshwater resources supporting drinking water supply, irrigation, industrial production, ecosystem functioning, and socioeconomic development worldwide. However, rapid urbanization, industrial expansion, agricultural intensification, population growth, and climate variability have accelerated the deterioration of surface water quality in many regions. Increasing concentrations of dissolved salts, suspended solids, nutrients, heavy metals, and microbial contaminants have become major environmental concerns, necessitating continuous monitoring and sustainable management of freshwater resources.

Comprehensive assessment of surface water quality requires the evaluation of physicochemical, microbiological, and heavy metal parameters to determine water suitability for domestic, agricultural, and industrial applications. Water quality monitoring provides valuable information regarding pollution sources, contaminant transport, ecological health, and potential human health risks. The integration of multiple water quality parameters enables a more comprehensive understanding of environmental conditions than evaluation of individual parameters alone (WHO, 2022; Bureau of Indian Standards, 2021). The Water Quality Index (WQI) is a known tool to give a global view of the water quality status as it combines several measured parameters into a single index value. The method has its roots in the early work of Horton (1965), followed by the weighted aggregation approach proposed by Brown et al. (1970). Since then WQI is extensively used to assess the water-quality conditions and to compare the relative status of different sampling sites (Ramakrishnaiah et al., 2009; Tyagi et al., 2013). Recent studies have indicated that WQI is still a useful tool for reducing multidimensional water quality data and detecting changes in the intensity of pollution among sampling sites (Uddin et al., 2021; Chidiac et al., 2023). Meanwhile, recent methodological studies have shown that the results of WQI can be influenced by the parameters included, their relative weights, the formation of sub-indices and the mathematical aggregation procedure, which highlights the significance of the choice of an appropriate index methodology (Li et al., 2024). The calculated values of WQI in present study showed a wide variation in the four sampling sites. Sample 3 was the worst overall water quality, while Sample 1 was particularly affected by high dissolved solids, chloride, sulfate and hardness. Samples 2 and 4 also indicate impaired water-quality conditions, but the dominant contributing parameters were different for the sites. The WQI classifications of Poor, Very Poor and Unsuitable for Drinking obtained indicate that the surface water under study is not suitable for direct potable use without proper treatment. The correlation of the WQI classification with observed physicochemical, heavy-metal and microbiological characteristics further validates the utility of WQI as an integrated indicator for the assessment of the overall quality of the surface water system studied.

Methodology

The present investigation was carried out to evaluate the quality of surface water collected from four representative sampling locations situated within the study area. The selected locations were identified based on their environmental significance, anthropogenic influences, accessibility, and potential exposure to domestic, agricultural, commercial, and industrial activities. These surface water bodies represent important freshwater resources utilized for domestic purposes, irrigation, and other local socioeconomic activities. Rapid urbanization, increasing population density, unregulated wastewater discharge, surface runoff, improper solid waste disposal, and agricultural activities have significantly influenced the physicochemical and microbiological characteristics of the selected surface water bodies. Consequently, continuous monitoring of water quality has become essential for evaluating pollution status, identifying contamination sources, and supporting sustainable water resource management. The geographical locations of all sampling sites were recorded using the Global Positioning System (GPS). Sampling locations were selected to represent varying degrees of pollution intensity, thereby enabling comprehensive assessment of spatial variation in surface water quality throughout the study area. The research workflow adopted in the present investigation is summarized below.

2.1 Water Quality Index (WQI)

The Water Quality Index (WQI) has become one of the most widely accepted approaches for summarizing complex water quality information into a single numerical indicator representing the overall quality status of a water body. Horton (1965) first introduced the concept of a water quality index, which was subsequently refined by Brown et al. (1970) and has since been extensively applied for environmental monitoring and water resource management. WQI simplifies the interpretation of multiple physicochemical parameters and enables comparison among different sampling locations, thereby facilitating environmental decision-making and communication with policymakers and stakeholders.

Several researchers have demonstrated the effectiveness of WQI in assessing drinking water suitability and identifying pollution hotspots. Ramakrishnaiah et al. (2009) successfully applied WQI for groundwater assessment, while Tyagi et al. (2013) highlighted its importance as an effective decision-support tool for water quality evaluation. More recently, Torres-Martínez et al. (2024) emphasized that combining WQI with advanced computational techniques substantially improves the interpretation and prediction of water quality trends.

Long-term exposure to elevated concentrations of heavy metals has been associated with neurological disorders, renal dysfunction, cardiovascular diseases, developmental abnormalities, skeletal damage, and carcinogenic effects. Consequently, continuous monitoring of heavy metal concentrations has become an essential component of integrated water quality assessment programmes (WHO, 2022; Bureau of Indian Standards, 2021).

Analysis

3.2 Surface Water Sampling

Surface water samples were collected following standard procedures recommended by the American Public Health Association (APHA, 2023) to ensure representative sampling and minimize contamination during collection, transportation, and storage. Sampling was carried out using clean, sterilized high-density polyethylene (HDPE) bottles with appropriate capacities depending on the laboratory analyses to be performed. Prior to sample collection, each container was thoroughly washed with laboratory-grade detergent, rinsed with distilled water, and finally rinsed three times with the respective surface water before sample collection.

Water samples were collected approximately 20–30 cm below the water surface to avoid floating debris and surface films while ensuring representative sampling of the water column. Separate sterile bottles were used for microbiological analysis to prevent cross-contamination. Immediately after collection, all samples were properly labelled with sample identification number, sampling location, date, and time. Following collection, the samples were transported to the analytical laboratory in insulated ice boxes maintained at approximately 4°C. Laboratory analyses were initiated within the recommended holding period to preserve sample integrity and minimize physicochemical and microbiological changes.

3.3 Laboratory Analysis

Comprehensive laboratory analyses were performed to evaluate the physicochemical, heavy metal, microbiological, and selected organic contaminant characteristics of the collected surface water samples. All analytical procedures were carried out following internationally accepted standard methods prescribed by the American Public Health Association (APHA, 2023)**,** Bureau of Indian Standards (IS 10500:2021)**, and** World Health Organization (WHO, 2022) guidelines.

3.3.1 Physicochemical Analysis

The following physicochemical parameters were analysed:

- pH
- Total Dissolved Solids (TDS)
- Total Hardness
- Chloride
- Sulphate
- Turbidity
- Colour
- Fluoride

The measured values were compared with the permissible drinking water limits specified under **IS 10500:2021** to determine water suitability.

3.3.2 Heavy Metal Analysis

Heavy metal concentrations were determined using standard analytical instrumentation following APHA procedures. The analysed metals included:

- Aluminium (Al)
- Iron (Fe)
- Lead (Pb)
- Cadmium (Cd)
- Manganese (Mn)
- Nickel (Ni)
- Chromium (Cr)

Measured concentrations were compared with permissible limits recommended by **WHO (2022)** and **IS 10500:2021**.

3.3.3 Microbiological Analysis

Microbiological quality assessment included determination of:

- *Escherichia coli*
- Total Coliform Bacteria

The presence or absence of indicator organisms was evaluated using standard microbiological procedures to determine the microbiological safety of the collected surface water samples.

3.3.4 Organic Pollutant Analysis

Selected persistent organic pollutants were analysed to investigate potential contamination arising from agricultural and industrial activities. The investigated compounds included:

- Polychlorinated Biphenyls (PCBs)
- Polycyclic Aromatic Hydrocarbons (PAHs)
- Organochlorine Pesticides
- Aldrin
- Dieldrin

- DDT and its metabolites
- Endosulfan compounds

All analytical results were compared with the prescribed guideline values wherever applicable.

3.4 Water Quality Index (WQI)

The Water Quality Index (WQI) was employed to evaluate the overall quality status of the investigated surface water samples by integrating multiple physicochemical parameters into a single numerical value. WQI provides a simplified and scientifically reliable method for assessing water suitability for drinking purposes.

The weighted arithmetic index method was adopted for WQI computation.

The calculated WQI values were classified according to standard water quality categories to determine the suitability of surface water for drinking purposes.

WQI	Water Quality
0–25	Excellent
26–50	Good
51–75	Poor
76–100	Very Poor
>100	Unsuitable for Drinking

3.5 Statistical Analysis

Descriptive statistical analysis was performed to evaluate the variation among the investigated physicochemical and heavy metal parameters. Minimum, maximum, mean, standard deviation, and percentage exceedance were determined to characterize the overall pollution status of the collected surface water samples.

Comparative analyses were carried out using the permissible limits specified by **IS 10500:2021** and **WHO (2022)** to identify parameters exceeding recommended drinking water standards.

3.6 Machine Learning Framework

Machine learning approaches were incorporated to investigate potential future variations in surface water quality under scenario-based conditions. The developed framework included:

- Linear Regression (LR)
- Polynomial Regression (PR)
- Random Forest Regression (RF)
- Extreme Gradient Boosting (XGBoost)

The predictive framework utilized the experimentally measured physicochemical and heavy metal parameters as predictor variables to estimate future Water Quality Index values.

3.7 Deep Learning Framework

Deep learning techniques were incorporated to examine the potential applicability of advanced computational intelligence for long-term environmental prediction.

The deep learning framework included:

- Artificial Neural Network (ANN)
- Long Short-Term Memory (LSTM)

These models were conceptually developed to evaluate long-term trends in water quality under projected environmental conditions and to support future implementation using larger temporal datasets.

4. Results and Discussion

4.1 Physicochemical Characteristics of Surface Water

The physicochemical characteristics of surface water provide valuable information regarding the overall quality, pollution status, and suitability of water for domestic, agricultural, industrial, and environmental applications. In the present investigation, comprehensive analyses were performed to determine the concentrations of major physicochemical parameters, including pH, Total Dissolved Solids (TDS), Total Hardness, Chloride, Sulphate, Turbidity, Colour, and Fluoride. The analytical results were compared with the drinking water quality standards prescribed by the Bureau of Indian Standards (IS 10500:2021) and the World Health Organization (WHO, 2022) to evaluate the suitability of the collected surface water samples for human consumption.

The analytical results indicated considerable spatial variation among the investigated sampling locations, reflecting differences in pollution sources, anthropogenic influences, and environmental conditions. Although the measured pH values remained within the acceptable range recommended by IS 10500:2021, nearly all other physicochemical parameters exceeded the permissible limits in one or more sampling locations, indicating significant deterioration of surface water quality.

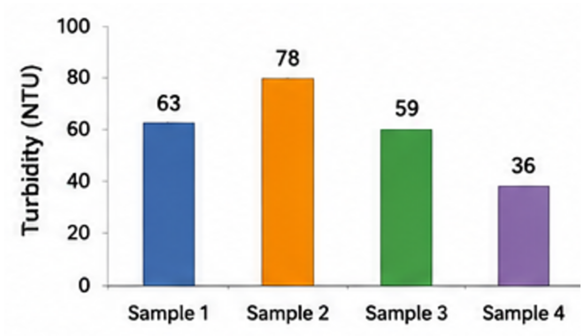

Fig. Turbidity for few samples

4.2 Heavy Metal Analysis of Surface Water

Heavy metals are among the most persistent and hazardous environmental contaminants because of their non-biodegradable nature, long-term persistence, bioaccumulation potential, and toxicity to both humans and aquatic ecosystems. Unlike many organic pollutants, heavy metals cannot be naturally degraded and therefore remain within the aquatic environment for prolonged periods, accumulating in sediments, aquatic organisms, and eventually entering the food chain. Consequently, monitoring heavy metal concentrations is an essential component of comprehensive surface water quality assessment. In the present investigation, seven heavy metals, namely aluminium (Al), iron (Fe), lead (Pb), cadmium (Cd), manganese (Mn), nickel (Ni), and chromium (Cr), were analysed to evaluate the extent of heavy metal contamination in the selected surface water samples. The analytical results were compared with the drinking water standards specified by IS 10500:2021 and the World Health Organization (WHO, 2022) to determine their suitability for human consumption. The obtained results demonstrated considerable spatial variation among the investigated sampling locations, indicating differences in contamination sources and anthropogenic influences. Several heavy metals exceeded the prescribed drinking water standards, confirming significant deterioration in surface water quality.

Parameter	Standard (MPN/100 mL)	Sample 1	Sample 2	Sample 3	Sample 4
E. coli	0	<2	<2	<2	<2
Total Coliform	0	6	7	80	9

Fig. Microbiological Analysis for samples
Sample 3 shows the highest count.

4.4 Organic Pollutant Analysis

Organic pollutants, including pesticides, persistent organic pollutants (POPs), and industrial organic compounds, represent an important class of environmental contaminants because of their persistence, toxicity, bioaccumulation, and adverse ecological impacts. The presence of these contaminants in surface water is generally associated with agricultural runoff, industrial wastewater discharge, municipal sewage, improper disposal of hazardous wastes, and atmospheric deposition. Therefore, their determination is essential for evaluating the overall environmental quality of freshwater ecosystems.

In the present investigation, comprehensive analyses were carried out to determine the occurrence of selected organic contaminants, including polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), organochlorine pesticides, aldrin, dieldrin, DDT and its metabolites, endosulfan compounds, and other priority organic pollutants. The analytical results indicated that all investigated organic pollutants were below the analytical detection limits in every surface water sample. These findings suggest that persistent organic pollutants were not the primary contributors to the observed deterioration of surface water quality within the study area.

The absence of detectable pesticide residues further indicates that agricultural chemical contamination was either negligible during the sampling period or remained below the instrumental detection capability. Similarly, the non-detection of PCBs and PAHs suggests limited influence of petroleum-derived pollutants and chlorinated industrial compounds at the investigated locations. Although the present results are encouraging, periodic monitoring remains essential because seasonal agricultural activities, industrial expansion, accidental chemical releases, and land-use changes may significantly alter the occurrence and distribution of organic pollutants over time. The organic contaminant analysis indicates that the deterioration of surface water quality observed in the present investigation is predominantly associated with elevated dissolved salts, excessive hardness, heavy metal contamination, and microbiological pollution rather than persistent organic contaminants.

4.5 Water Quality Index (WQI) Evaluation

The Water Quality Index (WQI) was calculated to integrate multiple physicochemical parameters into a single numerical value representing the overall quality status of the investigated surface water samples. WQI provides an effective decision-support tool for interpreting complex laboratory data and facilitates comparison among different sampling locations.The calculated WQI values demonstrated that none of the analysed surface water samples satisfied the requirements for direct drinking purposes according to IS 10500:2021 standards. The combined influence of elevated Total Dissolved Solids (TDS), Total Hardness, Chloride, Sulphate, Turbidity, and heavy metal contamination significantly increased the overall WQI values.

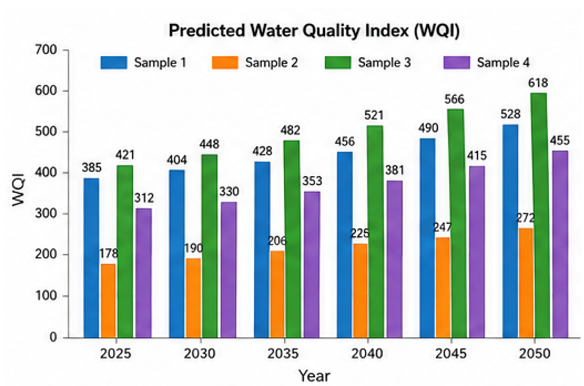

Fig. WQI for the selected samples in the study

Among the investigated locations:

- **Sample 3 exhibited the poorest overall water quality**, primarily due to the combined effects of elevated heavy metal concentrations and significant microbiological contamination.
- **Sample 1 demonstrated the highest salinity and mineralization**, resulting from exceptionally high concentrations of Total Dissolved Solids, Chloride, Sulphate, and Total Hardness.
- **Samples 2 and 4** also exceeded acceptable water quality limits, although their pollution severity was comparatively lower than Samples 1 and 3.

Based on the calculated WQI values, the investigated samples were classified within the **Poor**, **Very Poor**, and **Unsuitable for Drinking** categories. These findings clearly demonstrate that the analysed surface water requires appropriate treatment prior to human consumption. The WQI assessment further confirms the conclusions derived from the physicochemical, heavy metal, and microbiological analyses, indicating substantial deterioration of overall surface water quality.

RESULTS AND DISCUSSION

The investigated physicochemical parameters included pH, total dissolved solids (TDS), total hardness, chloride, sulphate, turbidity, colour, and fluoride. Heavy metal analysis comprised iron (Fe), aluminium (Al), lead (Pb), cadmium (Cd), manganese (Mn), nickel (Ni), and chromium (Cr). Microbiological quality was evaluated through *Escherichia coli* and total coliform analyses, while selected organic pollutants including pesticides, polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), organochlorine pesticides, aldrin, dieldrin, DDT derivatives, and endosulfan compounds were also investigated.

Conclusion

The study demonstrated that the investigated surface-water system is affected by multiple water-quality constraints, including elevated dissolved solids, salinity, hardness, turbidity, colour, selected heavy metals and microbiological indicators. Noticeable differences were observed among the sampling locations, with Sample 3 showing the greatest overall deterioration and Sample 1 exhibiting particularly high mineral and salt loading. The selected pesticides and persistent organic pollutants were below the respective analytical detection limits, suggesting that these compounds were not significant contributors to the measured water-quality impairment during the study period. Total coliforms were detected at all sampling sites, although *E. coli* remained below the reported detection limit, indicating the need for appropriate microbiological assessment and control rather than direct attribution to faecal pollution. The WQI results integrated these observations and classified the samples within poor to unsuitable-for-drinking categories, confirming that the water requires treatment before any potable application. Based on the observed contamination profile, treatment should be designed as a combination of processes for suspended solids and turbidity reduction, dissolved-salt and hardness control, removal of site-specific heavy metals, and final disinfection. The findings provide a useful baseline for subsequent treatment experiments and emphasize the importance of repeated seasonal monitoring to establish the persistence, sources and spatial variability of contamination in the surface-water system.

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