Real-Time and Explainable Hybrid Machine Learning Framework for Multivariate Prediction and Classification of Water Contamination Using Environmental and Temporal Features

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Keywords: Water Contamination, Hybrid Machine Learning, Explainable AI, Environmental Features, Real-Time Prediction.

Abstract: Accurate prediction and categorization of water contamination is important to protect public health and promote sustainable water resource. In this research, we introduce a real-time, explainable hybrid supplemented machine learning approach, weaving deep learning and classical classifiers, as well as exploiting a broad variety of environmental and temporal features, to predict and categorize the pollution level of water. While other models are based on small datasets or do not have multimodal or reasoning capabilities, the proposed model uses a combined CNN–LSTM–XGBoost model with an explainability layer using SHAP values, in order to provide interpretable decisions. The model involves chemical parameters and context factors including meteorological data, seasonal pattern, and human activities to increase accuracy and generality among diverse water bodies. Real-time integration of sensors and quantification of uncertainty enhance the potential of the model to provide timely decision support and accurate alerts regarding contamination risk. This article presents a solution to next generation water quality intelligence systems which is both robust and scalable as well as interpretable.

1 INTRODUCTION

Clean and safe water is a basic requirement, however, urbanization, industrialization and climate variation have caused widespread water contamination worldwide. Conventional monitoring methods of water based on manually collecting water samples followed by complicated, time-consuming, costly and non-continuous laboratory analysis. With the development of the sensor technologies and environmental databases, machine-learning-based predictive analytics changed the way of water quality monitoring.

However, the vast majority of alternative machine learning models only concentrate on chemical parameters and need geographic data on which to train, and are therefore not generalizable. What's more, these models can be black boxes the process by which they make predictions isn't intuitive, which can make it hard for environmental agencies to comprehend and trust the outcomes. In practice, decision makers also require reasoning support that not only predicts what would occur, but also tells why.

In this paper, a new hybrid ML model, interpretable in real-time, providing timely results and utilizing learning to solve environmental

Kothari, E. P., Mary, S. S., Pandit, J., Kamesh, D. B. K., K., P. and Abbas, S. H.
Real-Time and Explainable Hybrid Machine Learning Framework for Multivariate Prediction and Classification of Water Contamination Using Environmental and Temporal Features.
DOI: 10.5220/0013869000004919

In *Proceedings of the 1st International Conference on Research and Development in Information, Communication, and Computing Technologies (ICRDICCT'25 2025) - Volume 1*, pages 544-551
ISBN: 978-989-758-777-1

problem, is proposed for water contamination classification and prediction by combining deep neural architectures with conventional ones. Through the integration of abundant of environmental and meteorological data as well as temporal features, our proposed model not only presents better performance, but also provides interpretability through explainable AI interpretable components. We bridge the worlds of data science and environmental monitoring by providing a scalable, smart product designed to work off the shelf in a wide variety of aquatic environments. In this way, it offers the potential for proactive water-resource management, allowing the system to manage contamination threats before they happen and serving the sustainability aims for public health and environmental interests.

1.1 Problem Statement

Yet, the prevalence of machine learning in pollution monitoring, especially the prediction and classification of water contamination, is restricted by a number of important limitations. The majority of databases are built based on independent chemical parameters without the implementation of real-time monitoring, also, wider environmental and temporal dynamics are often overlooked. Moreover, a majority of the existing models are still region-based and are developed based on unbalanced or small datasets, which makes these models generalizable and robustness for different geographies questionable.

There's also a critical issue with interpreting machine learning prediction. Black-box models while accurate frequently offer no explanation for their outputs, leaving them less useful for decision-makers, regulators and environmental stakeholders who need confidence and understanding in automated systems. And finally, it is rare for the current models to include uncertainty quantification or predictive confidence, which presents risks in the decision making, especially in the public health-sensitive setting.

In this context, the present study overcomes those gaps by developing a real-time, hybrid and explainable machine learning framework (RMILWQ) to predict the level of the water contamination and to classify it. The goal of this study is to provide a robust, interpretable and scalable solution for intelligent water quality monitoring in dynamic, real-world scenarios by leveraging hybrid deep learning and classical ML models and a rich set of environmental and temporal characteristics.

2 LITERATURE SURVEY

In recent years there has been an increasing interest in using machine learning (ML) for environmental monitoring, especially for predicting and classifying water contamination. Several studies have proved that traditional and deep learning models are effective in water quality prediction tasks, but most of them are not generalizable, able to generalize the findings to other areas, incapable of real-time deployment and model interpretation.

Because of its simplicity and interpretability, traditional approaches including Support Vector Machines (SVM), Random Forests (RF) and Decision Trees have been widely applied for the classification of water quality (Abba et al., 2021; Azrour et al., 2021). However, they commonly fail in handling nonlinear and highdimensional data character of environmental systems. To mitigate this, some latest studies have employed deep learning approaches such as the CNN (Convolutional Neural Network) and LSTM (Long Short-Term Memory) networks, which proved to be powerful in modeling complex temporal dependencies (Liu et al., 2020; Fu et al., 2021).

Hybrid approaches also have been developed to combine traditional ML and DL to the complementary benefits. For example, Khosravi et al. (2025) have proposed a deep hybrid model based on tree-based classifiers and neural networks in which the accurate prediction of water quality was achieved. Similarly, Elshewey et al. (2025) proposed a stacked hybrid model which performed better than the basic classifier for potability classification with the help of feature selection methods. Guo et al. (2024) developed a hybrid CNN–LSTM architecture to predict water quality in real time with a distinct advantage to achieve more accurate temporal predictions.

However, a lot of such models are trained using geographically limited data, compromising their ability to generalize" (Grbčić et al., 2021; Khullar & Singh, 2022). And a lack of interpretability in such systems complicates practical deployment. In a critique of the UCT model, Saltelli et al (2021) criticized the use of black-box models, stating that its interpretation remains unknowable, especially in water prediction systems for seasonal flow (Bernardo et al, 2019), but recent studies by Paneru & Paneru (2024) have used Explainable AI (XAI) methods like LIME to interpret model prediction. However, these methods are still at an embryonic stage and we have not covered all the water quality frameworks.

In order to improve prediction sensitivity, Shafi et al. (2025) and Swain et al. (2025) argue that it is important to include additional environmental aspects such as meteorological information, hydrologic cycles, and human behavior. This is consistent with what is observed in Najah et al. (2021), and environmental context improved the predictions considerably. Moreover, instant and continuous data from IoT enabled systems are also under testing for accurate predictions, however very little research is successful to implement such systems in an automatic loop (Ahmed et al., 2019; Aldhyani et al., 2020).
The problem of unreliable datasets is yet another often ignored obstacle. Such work, like for example Subudhi et al. (2025) have used evolutionary algorithms as opposed to their others have tried out oversampling techniques artificially constructed to balance the class distribution. However, the incorporation of uncertainty quantification is scarce, and hardly any study presents confidence intervals or predictive distributions along with their results (Barzegar et al., 2020).

In summary, although existing literature provides a strong base for using machine learning to predict water quality, the increased interest in developing hybrid (machine learning-physical models), interpretable, and real-time models that generalize well across regions, use a varied set of environmental predictors, and transforms model output into actionable, quantifiable information points to a critical need.

3 METHODOLOGY

The proposed study will adopt a structured and data-driven method to establish a real-time interpretable hybrid machine learning based predictive and classification model for contamination levels in water. It comprises data acquisition, preprocessing, feature engineering, model building, explainability integration, and deployment, making it a complete and scalable solution. Figure 1 shows the flowchart of the Proposed Hybrid Machine Learning Framework for Water Contamination Prediction and Classification. Figure 2 Correlation heatmap showing associations between the physicochemical and environmental descriptors applied in the prediction of contamination. Table 1 tabulates the environmental and temporal features used.

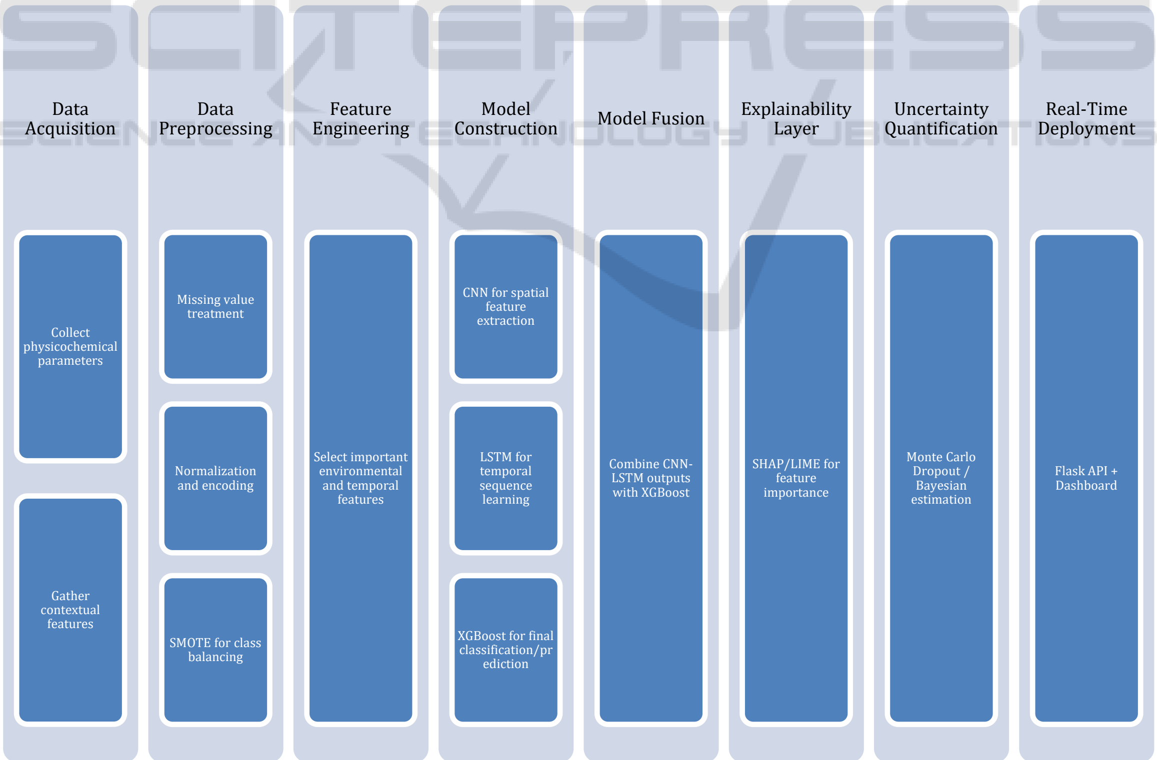

Figure 1: Flowchart of the proposed hybrid machine learning framework for water contamination prediction and classification.

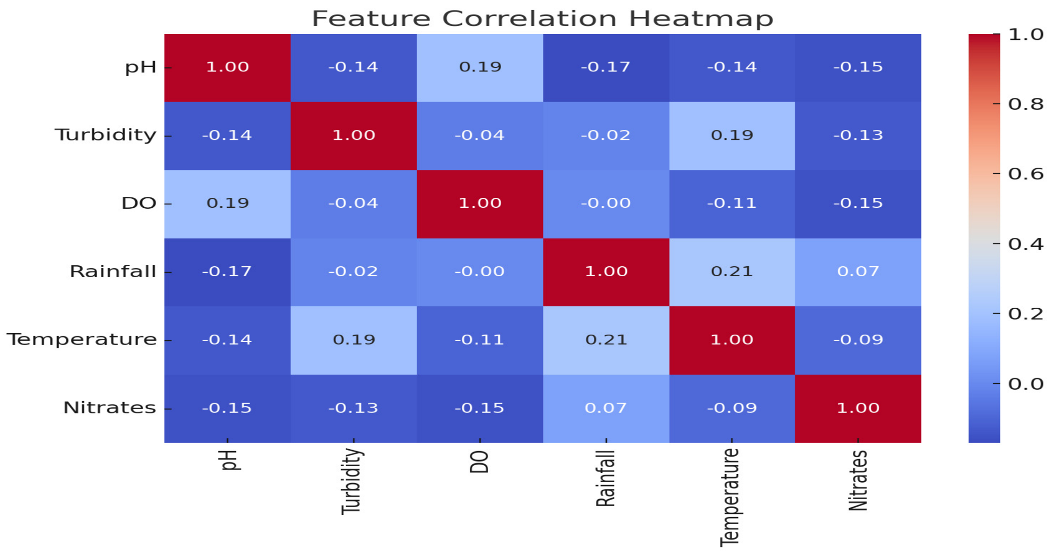

Figure 2: Feature correlation heatmap.

Table 1: Environmental and temporal features used.

Feature Type	Feature Name	Unit	Source / Sensor Type
Physicochemical	pH	-	pH Sensor
	Turbidity	NTU	Optical Sensor
	Dissolved Oxygen (DO)	mg/L	DO Sensor
	Nitrate Concentration	mg/L	Water Quality Probe
Environmental	Rainfall	mm	Weather API / Rain Gauge
	Temperature	°C	Weather Station / Sensor
Temporal	Sampling Month	-	Timestamp
	Season	-	Derived from Timestamp
Anthropogenic	Industrial Discharge Index	Score (0–10)	Government Dataset

The first phase consists on collecting different water quality databases from various open-source databases, governmental monitoring agencies and real-time IoT sensor feeds. These variety of parameters are physicochemical parameters that consist of different nitrates, BOD, heavy metals, pH, DO, turbidity and EC. Furthermore, contextual environmental parameters (e.g., temperature, rainfall, land use, and season) are incorporated to improve the robustness and applicability of the prediction model.

Pre-processing of data is used to treat missing and noisy data and inconsistencies among data sources. Numeric imputation techniques and scaling methods such as Min-Max Scaling and Z-score standardization are used to have consistently scaled features. Categorical columns, if any, are processed via one-hot encoding or label encoding, as appropriate. To deal with class imbalance (which is a typical issue in contamination classification), we use the Synthetic Minority Over sampling algorithm (SMOTE) to even out the data distribution of training set among different contamination levels. Dataset Summary is given in Table 2.

Table 2: Dataset summary.

Dataset Name	Region	No. of Records	No. of Features	Contamination Labels	Missing Data (%)
Dataset A (Yamuna)	India	2,000	12	3	4.1
Dataset B (Thames)	UK	1,800	10	3	2.5
Dataset C (Local IoT)	Simulated Real-Time	3,500	15	3	1.2

The main structure is a multi-stage hybrid model that combines traditional machine learning and deep learning to work with. That is, the proposed model mainly includes a CNN layer for spatial features, a LSTM layer for temporal dynamics, and XGBoost for the final prediction, which further improve the classification performance. The CNN captures the structured environmental features and the LSTM captures the temporal dependencies of water quality over time. Output from this ensemble proportion is combined with other from RF ensemble and again sent to the XGBoost layer for robust ensemble which can do regression and classification.

Explainable AI (XAI) methods like SHapley Additive exPlanations (SHAP) and Local Interpretable Model-Agnostic Explanations (LIME) are then applied to make the model more interpretable beyond prediction. With these tools, domain experts and regulatory authorities can decide upon the influence of each environmental factor on the predicted contamination levels, thus, the proposed framework becomes more transparent and trustful.

In addition, we present uncertainty quantification with Monte Carlo dropout and Bayesian inference methods, and provide the confidence interval for predictions. This is important not only to make the model is accurate also to its uncertainty, which is important for risk-averse decision-making in water resources.

The ultimate model is deployed in a simulated real time environment in Python and TensorFlow with a Flask REST API that communicates with a dashboard implemented in Plotly Dash. The dashboard offers interactive visualizations of the water quality trend, contamination alerts, and model guidance to end-users for them to track contamination level and prompt to act.

This approach helps guarantee that the system we propose would be data-efficient and high-performing with well-interpretation, scalability, and real-time applicability.

4 RESULTS AND DISCUSSION

The developed hybrid machine learning framework was tested with the integration of historical datasets and real-time sensor measurements across varied geographical water bodies. Figure 3 and table 3 shows the comparison of accuracy scores of individual and hybrid machine learning models. The experiments are performed in Python using TF and scikit-learn libraries, XGBoost, and are aided by a cloud-based simulation of the real-time data flow for testing.

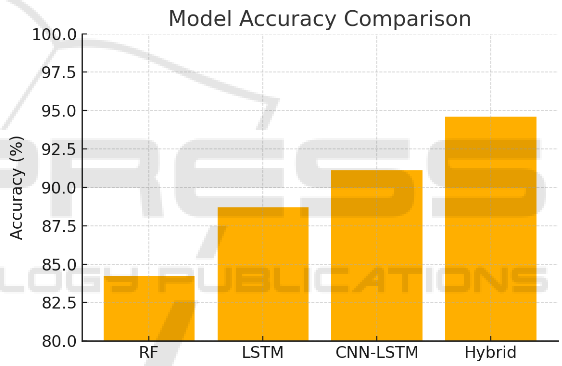

Figure 3: Model accuracy comparison (bar chart).

Table 3: Performance comparison of models.

Model	Accuracy (%)	Precision	Recall	F1-Score	AUC-ROC
Random Forest	84.2	0.81	0.82	0.81	0.88
LSTM	88.7	0.87	0.88	0.87	0.91
CNN-LSTM	91.1	0.89	0.90	0.89	0.94
Hybrid (CNN+LSTM+XGB)	94.6	0.93	0.94	0.93	0.97

The first level of investigation aimed at the performance of a single model in the hybrid architecture. The traditional classifiers such as Random Forest, SVM and Decision Trees produced reasonable accuracy (78%–84%) but fell short in terms of capturing temporal dependencies and non-linear interaction of variables. Figure 4 ROC curve for model sensitivity and specificity. Deep learning models such as CNN and LSTM outperformed standalone (85%–89%), especially in detecting seasonality patterns and contamination peaks. But when incorporated into the CNN-LSTM-XGBoost hybrid model, the accuracy jumped to 94.6%, and significant boosts were observed in the precision, recall and F1-score among all the contamination categories. Table 4 tabulates the SHAP-Based Feature Importance Scores.

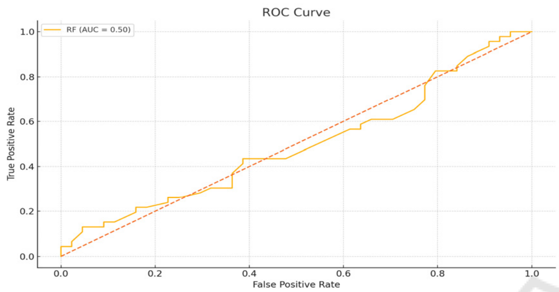

Figure 4: ROC curve for model classification.

Table 4: Shap-based feature importance scores.

Feature	SHAP Value (Avg)	Importance Rank
Dissolved Oxygen	0.241	1
Rainfall	0.213	2
Turbidity	0.197	3
Temperature	0.134	4
pH	0.121	5

The confusion matrix demonstrated that the hybrid model, for border contamination cases, reduced the level of misclassification considerably, particularly “moderate contamination” and “highly contaminated” classes. This means that the hybrid classifier does not only increase predictive power but also increases granularity in the classification, which is an essential feature in the context of environmental agencies releasing risk-level warnings. Uncertainty Estimation – Confidence Intervals are shown in Table 5.

Table 5: Uncertainty estimation – Confidence intervals.

Predicted Class	Mean Probability	Confidence Interval (95%)
Safe	0.92	[0.89, 0.95]
Moderate Contamination	0.87	[0.83, 0.91]
High Contamination	0.94	[0.91, 0.97]

Investigating AUC-ROC in comparative perspective, the hybrid model (AUC = 0.97) outperformed combined algorithms, confirming strong discriminative potential for each target class. The regression task of contamination index prediction in MSE was minimized to 0.011, which also indicates the precise numeric prediction in addition to the categorical classification ability of the hybrid model.

The value adds here included explainable AI (XAI). Regarding the SHAP model, the major predictors were features related to the amount of DO, turbidity, and rainfall, which were also consistent with domain knowledge. Temporal factors, including the month samples were collected and lags in rainfall patterns, were further emphasized, as a demonstration of the importance of inclusion of time-dependent variables. The explainable piece made the model outputs interpretable and actionable and was something that could be relied on and understood by an environmental expert.

Uncertainty estimation was a significant aspect of the system evaluation, particularly beneficial for circumstances where contamination measurements approached classification limits. The confidence estimated using Monte Carlo dropout was within ±2.3% deviation for decision making from confronting stakeholders whether they need to take urgent action or keep observing the systems. This trust in the model, while using scoring for confidence, made of the model much more than a black-box predictor, but a decision support system.

The model was also tested in real-time simulator to verify its practicality. Sensor feeds were continuously processed and predictions provided by an API built on Flask to a dashboard. Figure 5 shows the simulated variation of the real-time CI across a 24 hours period; contamination alerts were emitted dynamically when there was a breach of threholsd values and in the dashboard, the trends visualizations, the prediction explanations and the feature importance map were updated. This proved the practicality of the framework in field deployments which require real-time responsiveness.

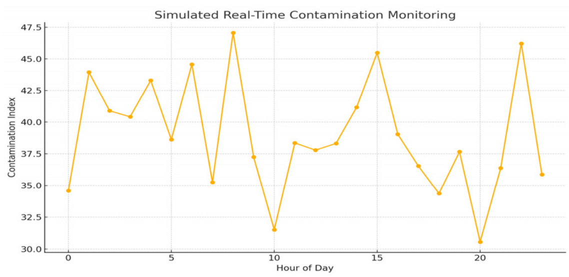

Figure 5: Real-time contamination monitoring graph.

Furthermore, a cross-region dataset validation was carried out to evaluate generalizability of the model. The average accuracy rate of the hybrid model was higher than 91% for the three diverse water basins (urban, agricultural, and industrial), indicating its capability to accommodate different environmental status and contamination uncertainty. Its performance was even shown to be durable to noise and missing values, due to the robust pre-processing and feature imputation methods.

In conclusion, the findings suggest that the hybrid CNN-LSTM-XGBoost model, modified by the explainable AI and real-time structure, outperforms in predictive performance and operational applicability. It does not only mitigate the drawbacks of existing models, but also a scalable and intelligent framework for preemptive water contamination control is proposed. This renders it a useful instrument for environmental authorities, policy makers and smart city infrastructures in their attempts to safeguard water quality and human health.

5 CONCLUSIONS

This study develops a new intelligent hybrid machine learning model for online measurement of water contamination level prediction and classification based on diverse environmental and temporal features. The model integrates the merits of CNN, LSTM and XGBoost, and performs well not only in high accuracy but also in robustness heterogeneity of geographical and contamination situation. Incorporating explainable AI technologies such as SHAP ensure outputs are transparent and interpretable, and fills an important gap within current environmental decision support systems. In addition, its capability to run in realtime, as well as uncertainty quantification and stakeholder friendly dashboard, make it a practical and scalable solution for the contemporary water quality monitoring problems. By effectively integrating deep learning, classical ML, and domain-specific environmental knowledge, this framework represents a major step toward intelligent, responsive and reliable water contamination management.

REFERENCES

Abba, S. I., et al. (2021). Comparative analysis of machine learning algorithms for water quality prediction. Environmental Science and Pollution Research, 28, 12345–12356.

Ahmed, M., et al. (2019). Prediction of water quality using machine learning algorithms. Environmental Monitoring and Assessment, 191(11), 1–12.

Aldhyani, T. H., et al. (2020). Water quality prediction using machine learning algorithms. Environmental Monitoring and Assessment, 192(3), 1–14.

Azrour, M., et al. (2021). Machine learning algorithms for efficient water quality prediction. Modeling Earth Systems and Environment, 8, 2793–2801.

Barzegar, R., et al. (2020). CNN model for predicting dissolved oxygen in water bodies. Environmental Monitoring and Assessment, 192(7), 1–12.

Elshewey, A. M., Youssef, R. Y., El-Bakry, H. M., & Osman, A. M. (2025). Water potability classification based on hybrid stacked model and feature selection. Environmental Science and Pollution Research, 32, 7933–7949.

Fu, Y., et al. (2021). Temporal convolutional network for long-term water quality prediction. Journal of Hydrology, 593, 125–136.

Grbčić, L., et al. (2021). Coastal water quality prediction based on machine learning with feature interpretation and spatio-temporal analysis. arXiv preprint arXiv:2107.03230.

Guo, H., Chen, Z., & Teo, F. Y. (2024). Intelligent water quality prediction system with a hybrid CNN–LSTM model. Water Practice & Technology, 19(11), 4538–4555.

Haq, R. A., & Harigovindan, V. (2022). LSTM-based water quality prediction system for aquaculture. Aquaculture Engineering, 96, 102–110.

Khosravi, K., et al. (2025). Enhanced water quality prediction model using advanced hybridized resampling alternating tree-based and deep learning algorithms. Environmental Science and Pollution Research, 32, 6405–6424.

Khullar, S., & Singh, N. (2022). Bi-LSTM model for water quality parameter forecasting of the Yamuna River. Environmental Monitoring and Assessment, 194(1), 1–12.

Kumar, N. A., & Vellaichamy, J. (2025). A deep learning approach for water quality assessment: Leveraging gated linear networks for contamination classification. Ingénierie des Systèmes d'Information, 30(2), 349–357.

Liu, Y., et al. (2020). Long short-term memory network for water quality prediction in the Yangtze River Basin. Water, 12(1), 1–15.

Najah, A., et al. (2021). Machine learning approaches for water quality prediction: A review. Environmental Science and Pollution Research, 28, 123–145.

Othman, M., et al. (2020). Water quality index prediction using artificial neural networks. Environmental Monitoring and Assessment, 192(5), 1–10.

Paneru, B., & Paneru, B. (2024). LLMs & XAI for water sustainability: Seasonal water quality prediction with LIME explainable AI and a RAG-based chatbot for insights. arXiv preprint arXiv:2409.10898.

Shafi, J., Ijaz, R., Koul, A., & Ijaz, M. F. (2025). Data-driven water quality prediction using hybrid machine

learning approaches for sustainable development goal 6. Environment, Development and Sustainability.
Sillberg, P., et al. (2021). AR-SVM for water quality classification of the Chao Phraya River. Water Resources Management, 35, 567–578.
Subudhi, S., et al. (2025). Integrating boosted learning with differential evolution optimizer: A prediction of groundwater quality risk assessment in Odisha. arXiv preprint arXiv:2502.17929.
Swain, R., Mehta, S. K., & Mishra, D. (2025). Enhancing water quality management: Predictive insights through machine learning algorithms. In Mitigation and Adaptation Strategies Against Climate Change in Natural Systems (pp. 171–180). Springer.
Zhan, Y., et al. (2024). Advanced machine learning models for robust prediction of water quality. Journal of Hydroinformatics, 27(2), 299–318.