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Machine Learning for Surface Water Quality Management in Malaysia: Integrating Physicochemical Parameters, Nutrient Loads, Land Use, Hydrological Conditions, and Anthropogenic Pressure

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ABSTRACT

Surface water quality in Malaysia is affected by urbanization, industrial expansion, agricultural activities, wastewater discharge, climatic variability, and changing hydrological regimes. This study conducted an empirical investigation of surface water quality in Malaysian river systems using measured water-quality data and machine learning analysis. A data-driven framework was developed and evaluated to assess water-quality conditions, predict variations, detect pollution events, and support river management. The analysis integrated physicochemical measurements with hydrological, spatial, land-use, and anthropogenic variables to examine spatial and temporal patterns and evaluate predictive performance. The investigated parameters include dissolved oxygen, biochemical oxygen demand, chemical oxygen demand, pH, temperature, electrical conductivity, turbidity, total suspended solids, ammoniacal nitrogen, nitrate, phosphate, total nitrogen, and total phosphorus, together with rainfall, streamflow, water level, antecedent rainfall, urbanization, agricultural land use, industrial land use, population density, wastewater pressure, and road density. Seven machine learning approaches are incorporated, including Decision Trees (DT), Random Forest (RF), Support Vector Machines (SVM), Support Vector Regression (SVR), Artificial Neural Networks (ANN), Long Short-Term Memory (LSTM) networks, and hybrid ensemble models. The Malaysian National Water Quality Standards and Water Quality Index (WQI) are incorporated to establish the regulatory and quantitative basis for water-quality classification and prediction. The framework further integrates explainable artificial intelligence techniques, including SHAP and LIME, to quantify predictor contributions and identify the dominant environmental and anthropogenic factors governing model outputs. The methodology integrated water-quality classification, continuous prediction, anomaly and pollution-event detection, identification of potential pollution pressures, and decision support for water-quality management. Particular emphasis is placed on temporal variability, nonlinear interactions, hydrological influence, land-use effects, and the integration of multiple environmental data sources. This study developed and evaluated a machine learning framework for surface-water quality assessment in Malaysia, integrating predictive modeling, model explainability, and watershed information to support conventional monitoring and the interpretation of water-quality patterns. The findings establish a methodological basis for developing real-time and transferable water-quality prediction systems capable of supporting pollution mitigation, watershed management, and sustainable water-resource planning across Malaysian river basins.

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1. Introduction

Surface water quality has been substantially affected during recent decades by the discharge of domestic wastewater [1], industrial effluents, agricultural pollutants, nutrients, suspended materials, organic contaminants, and other wastes [2]. Deteriorating water quality creates risks for human health, aquatic biodiversity, ecosystem functioning, water supply, irrigation, fisheries, and other beneficial uses [3,4,5]. The problem becomes more complex when climate variability modifies rainfall patterns, river discharge, water temperature, dilution capacity, and pollutant transport [6,7].

Sustainable surface-water management therefore requires systematic identification of the principal pollution sources and environmental pressures affecting rivers and other freshwater systems [8,9]. Traditional water-quality management relies heavily on periodic field sampling and laboratory analysis [10]. Although these procedures provide reliable measurements, their temporal and spatial coverage may be insufficient for rapidly changing pollution conditions [11]. Real-time sensors can improve temporal resolution, but their deployment can involve substantial acquisition, maintenance, calibration, and data-quality requirements [12].

Machine learning (ML) provides an alternative or complementary approach because it can identify nonlinear relationships among multiple environmental variables and transform large monitoring datasets into predictions, classifications, and early-warning information [13]. Previous research has demonstrated ML applications in water-quality classification, water-quality prediction, anomaly detection, pollution-source identification, and hydrological forecasting [14,15].

Malaysia provides a particularly relevant setting for this development. The Department of Environment (DOE) operates a national framework for river-water-quality standards and the River Water Quality Index [16]. Malaysian river waters are classified into Classes I, IIA, IIB, III, IV, and V according to designated uses and water-quality conditions [17]. Class I includes conservation and very limited-treatment uses, while Classes II–V correspond to progressively different treatment, fishery, recreational, livestock, irrigation, and other uses [18].

The Malaysian WQI framework also provides a direct basis for machine-learning classification. According to DOE documentation, WQI values of 81–100 are classified as clean, 60–80 as slightly polluted, and 0–59 as polluted [19]. The Malaysian classification framework incorporates parameters including ammoniacal nitrogen, biochemical oxygen demand, chemical oxygen demand, dissolved oxygen, pH, and total suspended solids [20].

Previous Malaysian research has already demonstrated the potential of ML for this purpose. Shamsuddin et al. developed ANN, Decision Tree, and Support Vector Machine models for multiclass water-quality classification in the Langat River Basin and reported that SVM provided strong classification performance [21]. Earlier research on the Langat River also combined chemometric techniques and ANN using extensive physicochemical measurements, identifying dissolved oxygen, BOD, pH, ammoniacal nitrogen, chlorine, E. coli, and coliform as important variables in explaining spatial water-quality variation [22].

However, a surface-water management system based only on conventional WQI parameters may not fully represent the processes controlling water quality. River condition is influenced not only by measured physicochemical properties but also by rainfall, discharge, catchment land use,

agricultural activity, industrialization, urban expansion, wastewater inputs, and population pressure. Therefore, a more comprehensive ML framework should integrate these variables [23].

This study empirically evaluated a machine learning framework for surface-water quality assessment in Malaysia using measured water-quality data and associated watershed variables. The analysis examined five dimensions—physicochemical conditions, nutrient loading, land use, hydrological conditions, and anthropogenic pressure—to assess their relationships with observed water-quality variations and their contributions to predictive performance.

The objectives are therefore to:

1. Evaluate the performance of selected machine learning algorithms for surface-water-quality assessment and prediction using the study dataset.
2. establish a Malaysia-oriented set of physicochemical, nutrient, hydrological, land-use, and anthropogenic variables;
3. integrate Malaysian WQI and national water-quality classes into an ML decision framework;
4. Evaluate and compare the predictive performance of DT, RF, SVM/SVR, ANN, LSTM, and ensemble models using the study dataset;
5. establish a framework for WQI classification, continuous water-quality prediction, and anomaly detection;
6. Apply explainable machine learning methods to quantify the contributions of environmental variables to model predictions and identify the most influential predictors; and
7. identify priorities for real-time, multi-source, and sustainable surface-water management in Malaysia.

2. Conceptual Framework for Surface Water Quality Management

2.1 Water Quality as a Multidimensional Environmental System

Water quality is a multidimensional concept involving physical, chemical, biological, and microbiological characteristics [24]. The conventional monitoring approach generally emphasizes direct measurements in water samples [25]. However, the observed value of a water-quality parameter can be influenced by hydrological conditions, upstream land use, pollution sources, meteorological conditions, and seasonal processes [26].

Consequently, the machine learning framework used in this study incorporated five interacting groups of variables to assess and predict surface-water quality [27,28,29,30]:

Group 1: Physicochemical parameters

- pH
- dissolved oxygen (DO)
- water temperature (WT)

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- electrical conductivity (EC)
- turbidity
- total suspended solids (TSS)
- total dissolved solids (TDS)
- biochemical oxygen demand (BOD)
- chemical oxygen demand (COD)

Group 2: Nutrient parameters

- ammoniacal nitrogen (NH_3-N)
- nitrate (NO_3^-)
- total nitrogen (TN)
- phosphate
- total phosphorus (TP)

Group 3: Hydrological and meteorological parameters

- rainfall intensity
- cumulative rainfall
- antecedent rainfall
- streamflow/discharge
- water level
- seasonal conditions
- antecedent dry period

Group 4: Land-use parameters

- urban/built-up land
- agricultural land
- industrial land
- forest land
- impervious-surface proportion
- road density

Group 5: Anthropogenic pressure

- population density
- wastewater discharge
- industrial intensity
- agricultural intensity
- urban expansion
- proximity to pollution sources

This structure allows ML models to move beyond a purely chemical description of water quality and toward a catchment-scale representation of pollution processes.

2.2 Water Quality Index and Classification

The Water Quality Index (WQI) [31] provides a numerical representation of overall water condition by integrating multiple parameters into a single index.

A general weighted formulation can be expressed as:

$$WQI = \frac{\sum_{i=1}^{n} q_i w_i}{\sum_{i=1}^{n} w_i}$$

where:

- q_i is the sub-index value of parameter i;
- w_i is the corresponding parameter weight; and
- n is the number of parameters.

The conventional WQI approach is useful because it transforms multiple measurements into a common management indicator. However, the calculation requires measurements for multiple parameters and may become computationally demanding when monitoring frequency and spatial coverage increase.

ML can complement this process by learning the relationship between available input parameters and WQI or WQI class. The model can subsequently estimate water-quality condition from a reduced or expanded set of observations.

Table 1. Malaysian Water Quality Index Classification

WQI range	DOE classification	General interpretation
81–100	Clean	Relatively good water quality
60–80	Slightly polluted	Moderate deterioration
0–59	Polluted	Significant pollution

Source: Malaysian Department of Environment water-quality classification.

Malaysia additionally uses Classes I, IIA, IIB, III, IV, and V to link water-quality conditions with designated uses[32].

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3. Machine Learning Algorithms for Surface Water Quality Management

3.1 Decision Tree

Decision Tree (DT) is a supervised-learning algorithm used for both classification and regression. It recursively divides observations according to selected predictor variables until terminal nodes representing predicted classes or numerical values are generated [33].

DT is particularly attractive for environmental applications because its decision structure can be interpreted comparatively easily. For example, a tree may identify combinations of low DO, high BOD, elevated ammoniacal nitrogen, and high TSS as conditions associated with degraded water-quality classes [34].

However, an individual tree can become excessively complex and overfit the training dataset. Pruning, cross-validation, and ensemble methods can therefore be used to improve generalization [35].

3.2 Random Forest

Random Forest (RF) combines multiple decision trees constructed using different bootstrap samples and subsets of predictor variables [36].

For water-quality management, RF has several advantages [37]:

1. ability to model nonlinear relationships;
2. capacity to accommodate many predictors;
3. relatively strong resistance to overfitting compared with individual trees;
4. ability to estimate variable importance;
5. suitability for classification and regression; and
6. applicability to mixed environmental datasets.

RF can therefore be used to predict WQI, classify water-quality classes, estimate individual pollutant concentrations, or identify the relative contribution of hydrological, land-use, and anthropogenic variables [38].

3.3 Support Vector Machine and Support Vector Regression

Support Vector Machine (SVM) is a supervised-learning method based on identifying an optimal decision boundary between classes. Kernel functions allow SVM to represent nonlinear relationships [39].

For continuous water-quality prediction, the corresponding Support Vector Regression (SVR) framework can be applied [40].

SVM/SVR is especially useful when [41]:

- datasets are relatively small;

- predictors are highly nonlinear;
- the number of variables is relatively high;
- generalization is important; and
- complex boundaries exist between water-quality classes.

A Malaysian study of the Langat River Basin demonstrated the applicability of SVM, ANN, and DT to multiclass WQI classification [42].

3.4 Artificial Neural Network

Artificial Neural Networks (ANNs) consist of interconnected computational nodes organized into input, hidden, and output layers [43].

For surface-water-quality management, ANN can learn nonlinear relationships between environmental variables and WQI or individual water-quality parameters [44].

For example:

$$WQI = f(D, O, B, O, D, C, O, D, p, HNH_3 - NTSSRainfallFlowLandUseAnthropogenicPressure)$$

The major advantage of ANN is its capacity to approximate highly nonlinear relationships [45]. However, ANN generally requires adequate training data, appropriate architecture selection, parameter tuning, and computational resources. Its internal decision process may also be difficult for environmental managers to interpret [46].

3.5 Long Short-Term Memory Networks

Water quality is inherently temporal. Measurements observed today may depend on conditions during previous hours, days, or weeks [47].

Long Short-Term Memory (LSTM) networks are a specialized form of recurrent neural network designed to learn temporal dependencies [48].

An LSTM-based framework can be represented conceptually as:

$$WQI_t = f(X_t, X_{t-1}, ., ..X_{t-k})$$

where $X_t$represents the environmental variables observed at time t, and $k$represents the historical time window.

Potential LSTM inputs include [49,50]:

- previous DO values;
- previous BOD/COD;
- rainfall;
- cumulative rainfall;

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- streamflow;
- water level;
- nutrient concentrations;
- temperature; and
- previous WQI.

This makes LSTM particularly relevant for early-warning systems.

4. Machine Learning Framework for Surface-Water Quality Assessment in Malaysia

The machine learning framework used in this study comprised six sequential stages.

Stage 1: Multi-source data acquisition

The data sources used in this study included:

- DOE monitoring stations;
- automated water-quality sensors;
- meteorological stations;
- hydrological stations;
- GIS databases;
- satellite-derived land-use products;
- population databases;
- industrial databases; and
- wastewater-discharge records.

Stage 2: Data preprocessing

The dataset underwent the following preprocessing procedures:

1. quality control;
2. missing-value treatment;
3. outlier identification;
4. temporal synchronization;
5. spatial matching;

6. normalization where required;
7. feature selection; and
8. class-balance assessment.

Stage 3: Feature integration

The five predictor groups were combined into a unified feature matrix for model development and evaluation.

Stage 4: Model development

The comparative analysis included at least four model families:

- DT;
- RF;
- SVM/SVR;
- ANN/LSTM.

Ensemble models were subsequently constructed by combining the best-performing individual models.

Stage 5: Model interpretation

SHAP and LIME were applied to quantify and interpret the contribution of each predictor to model predictions.

Stage 6: Management application

The final system generated the following outputs:

- WQI;
- water-quality class;
- pollutant predictions;
- anomaly alerts;
- pollution-pressure indicators; and
- management recommendations.

5. Study Variables and Their Environmental Roles

Table 2. Integrated predictor framework

Dimension	Variables	Expected	management

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		relevance
Physicochemical	pH, DO, WT, EC, turbidity, TSS, TDS	Direct representation of water condition
Organic pollution	BOD, COD	Organic and chemical pollution
Nutrients	NH_3-N, NO_3^-, TN, phosphate, TP	Nutrient enrichment and eutrophication
Hydrology	rainfall, discharge, water level	Pollutant dilution and transport
Climate	temperature, rainfall intensity, antecedent rainfall	Seasonal and event-driven changes
Land use	urban, agriculture, forest, industrial	Spatial pollution pressure
Urbanization	built-up area, impervious surface	Runoff and pollutant loading
Anthropogenic	population density, wastewater, industrial intensity	Human-generated pressure
Transport	road density, drainage connectivity	Pollutant mobilization
Management	WQI, WQC class	Final management indicators

The principal methodological contribution of this study was the integration of water chemistry and catchment-scale environmental drivers within a unified machine learning framework for water-quality assessment and prediction.

6. Machine Learning for Water-Quality Classification

Water-quality classification is one of the most established ML applications in surface-water management.

The classification model was used to estimate:

$$Y \in \{C, l, eanSlightly\ PollutedPolluted\}$$

or, at the Malaysian regulatory level:

$$Y \in \{I, I, I, A, I, IBIIIIVV\}$$

The input vector can contain both conventional water-quality parameters and contextual environmental variables.

Table 3. Classification Models Evaluated in This Study

Model	Main application	Major advantage	Main limitation
DT	WQI classification	Easy interpretation	Overfitting
RF	Multiclass WQI	Robust nonlinear modeling	Lower transparency
SVM	WQI classification	Strong nonlinear classification	Parameter tuning
ANN	Complex classification	Nonlinear learning	Requires sufficient data
KNN	Similarity classification	Simple implementation	Sensitive to scale/outliers
XGBoost	Ensemble classification	High predictive capacity	Hyperparameter complexity
LSTM	Temporal	Learns temporal dependence	Data and computational

	classification		demand

Existing Malaysian evidence supports the feasibility of this approach. Research in the Langat River Basin used ANN, DT, and SVM for multiclass water-quality classification, while other Malaysian work has investigated ANN-based WQI prediction.

7. Machine Learning for Continuous Water-Quality Prediction

Classification alone does not provide sufficient information for proactive management. Environmental agencies also require estimates of future pollutant concentrations and WQI.

A continuous prediction model can be formulated as:

$$\hat{Y}_{t+h} = f(X_t, X_{t-1}, \ldots X_{t-k})$$

where:

- $\hat{Y}_{t+h}$is the predicted water-quality variable;
- $h$is the prediction horizon;
- $X_t$is the current environmental state; and
- $k$represents historical observations.

The prediction targets evaluated in this study included:

- DO;
- BOD;
- COD;
- NH_3-N;
- NO_3^-;
- TP;
- TSS;
- turbidity;
- WQI; and
- water-quality class.

The inclusion of hydrological variables is particularly important because rainfall and discharge can alter pollutant concentration through dilution, mobilization, and transport.

8. Nutrient-Load Modeling

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Nutrient pollution represents an important extension of conventional WQI-based modeling[51].

Nitrogen and phosphorus can originate from[52]:

- agricultural fertilizers;
- livestock operations;
- domestic wastewater;
- industrial wastewater;
- urban runoff;
- soil erosion; and
- atmospheric deposition.

The machine learning framework used in this study therefore incorporated:

$$N_{load} = f(N, H_3, -, N, N, O_3^- TNRainfallFlowLandUse)$$

and

$$P_{load} = f(P, O_4^{3-}, T, P, RainfallFlowLandUse)$$

These relationships can be used to identify periods and locations where nutrient loading is likely to increase.

Importantly, concentration and load should not be treated as identical variables. Concentration describes pollutant abundance per unit water volume, whereas load incorporates flow and therefore provides information about the total pollutant mass transported through a river system[53].

9. Land Use and Spatial Water-Quality Modeling

Land use determines the spatial distribution of many pollution pressures[54].

Urban areas may contribute[55]:

- road runoff;
- suspended solids;
- metals;
- hydrocarbons;
- nutrients; and
- wastewater-related pressures.

Agricultural areas may contribute[56]:

- nitrogen;

- phosphorus;
- pesticides;
- sediments; and
- organic matter.

Industrial areas may contribute[57]:

- chemical pollutants;
- metals;
- organic contaminants; and
- elevated thermal or conductivity signals.

Forested areas generally represent a different hydrological and pollution-pressure regime[58].

Accordingly, GIS-derived land-use variables were incorporated into the machine learning models to account for the environmental context of each monitoring station and the influence of surrounding watershed characteristics.

The spatial features incorporated into the analysis included:

$$UrbanRatio = \frac{A_{urban}}{A_{catchment}}$$

$$AgriculturalRatio = \frac{A_{agriculture}}{A_{catchment}}$$

$$IndustrialRatio = \frac{A_{industrial}}{A_{catchment}}$$

and:

$$ImperviousRatio = \frac{A_{impervious}}{A_{catchment}}$$

These variables can be calculated for different buffer distances around monitoring stations or upstream subcatchments.

10. Hydrological Conditions and Water Quality

Hydrology provides an essential link between pollution sources and observed water quality[59].

Rainfall can increase surface runoff and transport pollutants from urban and agricultural surfaces into rivers. Conversely, prolonged low-flow conditions can reduce dilution capacity and increase the concentration of some pollutants[60].

The framework implemented in this study therefore incorporated:

- current rainfall;

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- cumulative rainfall;
- 24-h rainfall;
- 72-h rainfall;
- antecedent precipitation;
- discharge;
- water level;
- flow velocity where available; and
- dry-period duration.

An antecedent rainfall index may be represented conceptually as:

$$API_t = P_t + kP_{t-1} + k^2P_{t-2} + \ldots + k^nP_{t-n}$$

where P_t is rainfall and k is a recession coefficient.

The inclusion of these variables allows the ML model to distinguish between pollution generated under normal flow and pollution mobilized during rainfall events.

11. Anthropogenic Pressure Index

A further extension of the framework is the construction of an Anthropogenic Pressure Index (API*) based on normalized human-pressure variables[61].

The mathematical formulation used in this study was expressed as follows:

$$API^* = \sum_{j=1}^{m} w_j Z_j$$

where Z_j represents a normalized anthropogenic-pressure variable and w_j represents its assigned or data-derived weight.

The components incorporated into the framework included:

- population density;
- industrial density;
- wastewater discharge;
- agricultural intensity;
- built-up proportion;
- road density; and

- proximity to wastewater outlets.

The purpose of this index is not to replace direct pollution measurements. Rather, it provides a contextual representation of human pressure that can improve spatial prediction and source interpretation.

12. Explainable Machine Learning

High predictive accuracy alone is insufficient for environmental decision-making. Managers need to know why a model predicts deterioration[62].

SHAP (SHapley Additive exPlanations) can quantify the contribution of individual variables to predictions[63].

For example, The SHAP analysis indicated that [64,65]:

- rainfall has a strong positive contribution to TSS;
- high BOD contributes negatively to WQI;
- elevated DO contributes positively to WQI;
- urban land proportion increases pollution probability;
- ammoniacal nitrogen strongly influences WQI class.

LIME can provide local explanations for individual predictions.

The framework used in this study therefore combined:

$$Prediction + Explanation + Environmental\ Interpretation$$

rather than prediction alone.

13. Water-Quality Anomaly Detection

Pollution incidents do not necessarily correspond to a gradual decline in WQI. Sudden changes can indicate[66,67]:

- accidental discharge;
- wastewater-system failure;
- intense storm runoff;
- illegal discharge;
- sensor malfunction; or
- unusual hydrological conditions.

Unsupervised ML can detect unusual observations without requiring a complete labeled database.

The methods used in this study included [68,69]:

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- Isolation Forest;
- One-Class SVM;
- clustering;
- autoencoders;
- Bayesian approaches; and
- LSTM-based temporal anomaly detection.

An anomaly score can be used to generate early warnings:

$$A_t = f\left(X_t - \hat{X}_t\right)$$

where $X_t$represents observed conditions and $\hat{X}_t$represents expected conditions.

14. Performance Evaluation

The models were evaluated using performance metrics appropriate to each prediction task.

For regression:

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |\, y_i - \hat{y}_i \,|$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$$

For classification:

- accuracy;
- precision;
- recall;
- F1-score;
- balanced accuracy;
- Cohen's kappa; and
- confusion matrix.

For imbalanced water-quality classes, accuracy alone should not be considered sufficient. Macro-F1 and class-specific recall should also be reported.

15. Validation Strategy

Random train-test splitting can produce overly optimistic results when environmental observations are temporally or spatially dependent.

Accordingly, the framework applied in this Malaysian study used:

Temporal validation

Training on earlier observations and testing on later observations.

Spatial validation

Training on some monitoring stations and testing on geographically separate stations.

Catchment-level validation

Training on selected catchments and testing on an independent catchment.

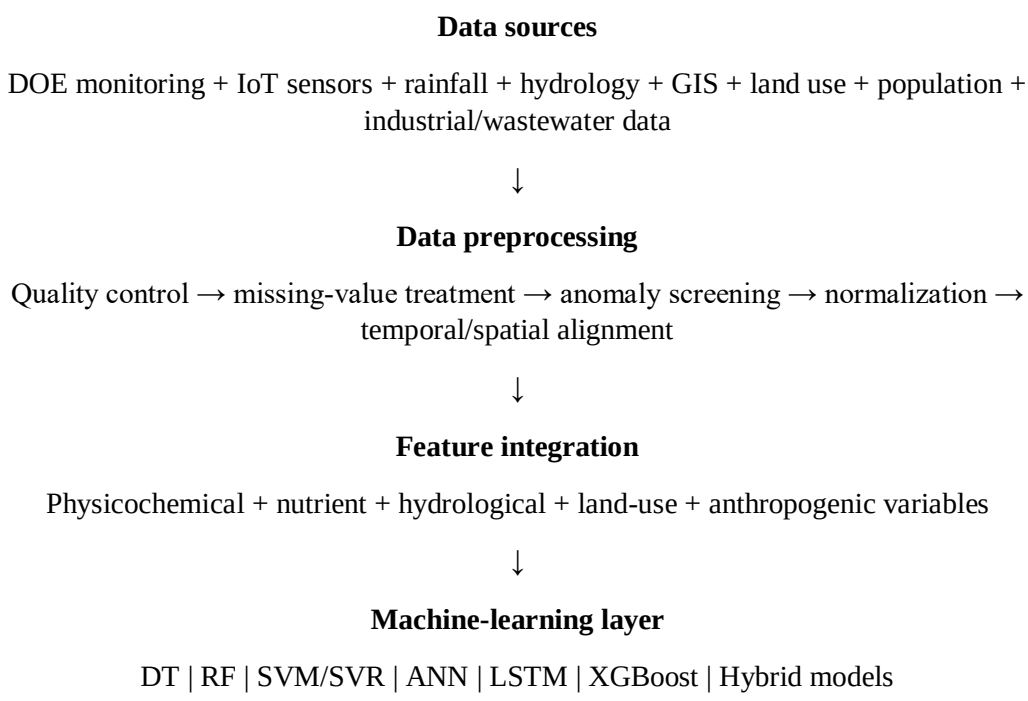
Extreme-event validation

Testing specifically during high-rainfall and unusual pollution episodes.

These procedures provide stronger evidence of whether an ML model can generalize beyond the data used for model development.

16. Integrated Decision-Support Framework

Figure 1. Architecture of the Machine Learning Framework Used for Surface-Water Quality Assessment in Malaysia



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↓

Outputs

WQI prediction + WQC classification + pollutant prediction + anomaly detection

↓

Explainability

SHAP + LIME + variable importance

↓

Management

Early warning + pollution-source prioritization + monitoring optimization + water-quality protection

17. Comparative Interpretation of Machine Learning Approaches

Table 4. Roles of machine learning models in the Malaysian surface-water quality framework.

Model	Classification	Regression	Time series	Explainability	Recommended role
DT	High	High	Low	High	Transparent baseline
RF	High	High	Moderate	Moderate–High	Main ensemble model
SVM	High	High	Moderate	Moderate	Small/medium datasets
ANN	High	High	Moderate	Low	Nonlinear relationships
LSTM	Moderate	High	Very high	Low	Temporal forecasting
XGBoost	High	High	Moderate	Moderate–High	High-performance tabular data
KNN	Moderate	Moderate	Low	High	Benchmark/similarity
Hybrid models	High	High	Very high	Variable	Advanced prediction

18. Evidence from Malaysian Applications

The methodological approach adopted in this study aligns with existing Malaysian research on machine learning applications in surface-water quality assessment.

The Langat River Basin has been used extensively as a Malaysian case for data-driven water-quality analysis. Earlier research analyzed 23 physicochemical parameters from seven monitoring stations and used multivariate techniques and ANN to distinguish pollution regions[70,71,72,73,74,75,76,77,78,79].

More recent research developed ANN, DT, and SVM models for multiclass WQI classification in the Langat River Basin. The study showed that ML can reduce the computational complexity

associated with conventional WQI classification and demonstrated the practical relevance of SVM-based classification.

Other Malaysian research has developed ANN models for WQI estimation in the Langat River, while ML studies have also investigated SVM-based water-quality prediction for catchments where direct observations may be limited.

These studies provide empirical support for applying machine learning to Malaysian river management. Building on this evidence, the present study integrated land-use, hydrological, nutrient-loading, and anthropogenic-pressure variables into the analysis to assess their contributions to water-quality prediction.

19. Advantages of the Study Framework

The integrated approach combines predictive modeling, model explainability, and watershed information to support surface-water quality assessment and management.

First, the framework incorporated contextual environmental information alongside conventional water-quality variables to broaden the basis of assessment.

Second, predictive modeling was used to estimate water-quality conditions between sampling events.

Third, spatial and temporal information was integrated to characterize variation across monitoring locations and periods.

Fourth, feature-importance and explainability analyses identified predictors associated with deteriorating water-quality conditions.

Fifth, pollution-event detection formed the analytical basis for early-warning applications.

Sixth, the framework supported the identification of locations and periods requiring additional sampling.

Finally, its application to other Malaysian catchments remains subject to local calibration and independent validation.

20. Limitations and Research Challenges

Several limitations should be considered when interpreting the study findings and assessing the applicability of the framework.

20.1 Data availability

ML performance depends heavily on the quantity, quality, temporal resolution, and representativeness of training data.

20.2 Missing observations

Environmental datasets frequently contain missing observations resulting from sensor failure, sampling interruptions, laboratory limitations, or changes in monitoring programs.

20.3 Spatial heterogeneity

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Different Malaysian catchments have different hydrological, geological, climatic, land-use, and anthropogenic characteristics. A model trained in one basin should therefore not automatically be assumed to generalize to another.

20.4 Concept drift

Water-quality relationships can change because of urban expansion, climate variability, wastewater-treatment improvements, industrial changes, or land-use conversion.

20.5 Black-box models

Deep-learning models can provide strong predictive performance while remaining difficult to interpret.

20.6 Data leakage

Variables used to calculate WQI should be carefully distinguished from independent predictors when evaluating ML models intended to predict WQI. Otherwise, performance may be artificially inflated.

20.7 Regulatory compatibility

ML outputs should complement rather than replace official Malaysian regulatory procedures unless formally validated and adopted by the relevant authorities.

21. Future Research Directions

Future Malaysian studies should focus on seven priorities.

21.1 Multi-source data fusion

The integration of DOE observations, IoT sensors, remote sensing, GIS, rainfall, hydrology, and socioeconomic data can produce a more comprehensive representation of catchment conditions.

21.2 Hybrid models

Hybrid architectures combining RF/XGBoost with LSTM or CNN-LSTM may be particularly useful for datasets containing both spatial and temporal patterns.

21.3 Explainable AI

SHAP, LIME, partial-dependence analysis, and feature-interaction analysis should become standard components of environmental ML studies.

21.4 Transfer learning

Models trained in data-rich Malaysian basins could potentially be adapted to data-limited basins through transfer-learning approaches, subject to rigorous validation.

21.5 Real-time monitoring

The integration of IoT sensors with ML could allow continuous water-quality assessment and automated warning generation.

21.6 Uncertainty quantification

Future models should provide prediction intervals rather than only point predictions.

21.7 Climate-change integration

Rainfall extremes, temperature changes, drought periods, and changing flow regimes should be incorporated into long-term water-quality prediction frameworks.

22. Management Implications for Malaysia

The framework developed in this study provides a basis for supporting environmental management at several levels.

At the **monitoring level**, ML can identify which variables and stations require more frequent measurements.

At the **operational level**, real-time models can provide early warnings.

At the **catchment level**, land-use and anthropogenic variables can identify areas where pollution pressure is concentrated.

At the **regulatory level**, predicted WQI and water-quality classes can provide supplementary information for prioritizing investigation.

At the **strategic level**, long-term models can evaluate relationships between urbanization, climate variability, nutrient loading, and river-water quality.

Malaysia's existing DOE standards provide an appropriate regulatory reference because they link water-quality measurements to water-use classes and WQI categories.

23. Conclusions

Machine learning has substantial potential to strengthen surface-water-quality management in Malaysia by transforming conventional monitoring data into classification, prediction, anomaly-detection, and early-warning systems.

The principal contribution of this study was the integration of five dimensions of environmental information within a machine learning framework: **physicochemical parameters, nutrient loads, land use, hydrological conditions, and anthropogenic pressure**. These variables were analyzed jointly to examine their relationships with observed river-water quality and assess their contributions to predictive performance. This approach incorporated information on pollution sources, catchment characteristics, hydrological processes, and human activities alongside water chemistry.

DT, RF, SVM/SVR, ANN, LSTM, and ensemble algorithms each have different strengths. Tree-based methods provide strong performance on heterogeneous tabular datasets and can offer useful feature-importance information. SVM can be effective for nonlinear classification and relatively limited datasets. ANN can represent complex nonlinear relationships, while LSTM is particularly suitable for temporal forecasting. Hybrid models may provide additional advantages when spatial, temporal, and nonlinear processes interact.

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The Malaysian regulatory context provides a strong foundation for ML development. The DOE framework uses WQI and water-use classes to characterize river-water quality, while existing Malaysian research has already demonstrated the feasibility of ANN, DT, SVM, and related approaches in the Langat River Basin.

The next generation of Malaysian water-quality ML systems should therefore move beyond models based solely on conventional WQI parameters. Integrating rainfall, streamflow, antecedent hydrological conditions, land-use composition, urbanization, agricultural activity, industrial pressure, population density, and wastewater information can provide a more complete representation of the mechanisms controlling surface-water quality.

At the same time, predictive accuracy should not be the only criterion for model selection. Explainability, uncertainty, spatial transferability, temporal robustness, data quality, regulatory compatibility, and operational feasibility are equally important. SHAP and LIME can help transform complex ML models into more interpretable decision-support tools by showing how individual environmental variables contribute to predictions.

A mature Malaysian surface-water ML system should ultimately connect **monitoring → prediction → explanation → early warning → management response**. Such an integrated architecture can complement conventional environmental monitoring, improve the efficiency of water-quality assessment, and provide a scientifically grounded foundation for proactive surface-water management.

The framework provides a methodological basis for analyzing Malaysian DOE monitoring records, IoT observations, hydrological datasets, remote-sensing products, and GIS-derived catchment characteristics. Further evaluation using independently collected Malaysian observations, including spatial, temporal, and event-based validation, is needed to establish model reliability and generalizability beyond the study dataset.

Ethical Considerations

Not applicable. This study did not require ethical approval because it does not include human or animal subjects and does not involve any personal or sensitive data.

List of Abbrevations:

(WQI): The Water Quality Index ; (ML): Machine learning;(DOE): Department of Environment; (DO): dissolved oxygen; (WT): water temperature ; (EC): electrical conductivity; (TSS): total suspended solids ; (TDS): total dissolved solids; (BOD): biochemical oxygen demand; (COD): chemical oxygen demand; (NH_3-N): ammoniacal nitrogen; (NO_3^-): nitrate; (TN): total nitrogen; (TP): total phosphorus; (DT) : Decision Tree; (RF) : Random Forest;(SVM): Support Vector Machine ; (SVR) : Support Vector Regression; (ANNs): Artificial Neural Networks; (LSTM): Long Short-Term Memory.

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Author Contribution:

All authors contributed equally to the main contributor to this paper. All authors read and approved the final paper.

Declaration of generative AI and AI-assisted technologies in the writing process

The authors hereby declare that no generative artificial intelligence or AI-assisted technologies were used at any stage during the preparation of this manuscript, including language editing, proofreading, or content development. The authors take full responsibility for the originality and integrity of the work presented in this publication.

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