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# Predictive Water Quality Assessment and Dye degradation potential by metal mediated GO/$H_2O_2$ Using Optimized Machine Learning Models

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***Abstract*--** **Water quality assessment requires the simultaneous evaluation of several physicochemical parameters, making conventional assessment methods time-consuming and difficult to interpret when multiple contaminants are present. The present study proposes an integrated approach combining water quality index (WQI), machine learning (ML), and graphene oxide (GO)-based treatment for water-quality assessment and pollutant removal. Water samples collected from selected locations were analyzed for pH, total hardness, fluoride, phosphorus, iron, nitrate, ammonia, residual chlorine and chemical oxygen demand (COD). The measured parameters were used to determine WQI and classify the samples according to their overall quality. Optimized machine learning models were employed to identify patterns among the physicochemical parameters and predict water-quality classes. The analysis identified fluoride, nitrate, ammonia, pH and COD as important parameters contributing to variations in water quality. Several samples showed elevated nitrate, fluoride, ammonia and COD levels, indicating the need for appropriate treatment before direct use. In addition, graphene oxide (GO) was investigated as a functional nanomaterial for water purification and dye degradation. The oxygen-containing functional groups of GO provide active sites for adsorption and interaction with dissolved pollutants. UV/oxidative dye-degradation experiments were performed using selected blue, violet and maroon dyes, and changes in absorbance were monitored at regular time intervals. The results demonstrated that dye degradation behaviour varied with dye type and treatment conditions. The combined ML-WQI and GO-treatment strategy provides a promising framework for rapid water-quality prediction, identification of contaminated sources, hardness/pollutant reduction and dye-contaminated wastewater treatment. The approach can support sustainable water-quality monitoring and the development of low-cost nanomaterial-based treatment systems.**

***Keywords*--** **Water Quality Index; Machine Learning; Artificial Intelligence; Graphene Oxide; Dye Degradation; Wastewater Treatment; Physicochemical Parameters; Water Purification.**

## I. INTRODUCTION

Water is an essential natural resource for human health, agriculture, industrial development and ecosystem sustainability. Increased urbanization, industrialization, agricultural activities and improper wastewater disposal have resulted in deterioration of water quality in many surface-water and groundwater systems. Water quality is generally evaluated using individual physicochemical parameters such as pH, total hardness, fluoride, nitrate, ammonia, phosphorus, iron, residual chlorine and chemical oxygen demand (COD). Although individual parameters provide useful information, interpretation becomes complicated when several parameters vary simultaneously. The Water Quality Index (WQI) provides a simplified numerical representation of overall water quality by integrating several physicochemical parameters into a single index. However, WQI calculations may depend strongly on the selected parameters, weighting factors and classification criteria.

Recent advances in artificial intelligence (AI) and machine learning (ML) provide new opportunities for environmental monitoring and water-quality prediction. Machine learning algorithms can identify nonlinear relationships between multiple water-quality parameters and water-quality classes. Optimized ML models can therefore assist in predicting water-quality status, identifying influential parameters and reducing the time required for conventional interpretation. However, model performance depends on data quality, sample size, parameter selection, preprocessing and appropriate model optimization.

Dye-containing wastewater is an important environmental concern because synthetic dyes are widely used in textile, printing, leather, pharmaceutical and related industries. Many dyes are chemically stable and can persist in aquatic environments.

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Their intense colour can reduce light penetration into water bodies, while some dye molecules and their degradation products may have adverse environmental effects. Therefore, the development of efficient and sustainable dye-removal technologies is important.

In the present investigation, GO was explored as a functional material for water purification and dye degradation, while ML models were used for water-quality assessment. Selected water samples were characterized using multiple physicochemical parameters, and WQI values were used as a basis for classification. AI/ML tools were then applied to identify patterns and predict water-quality status. In parallel, selected synthetic dyes were subjected to GO-assisted/oxidative treatment under controlled experimental conditions, and their degradation behaviour was monitored spectrophotometrically.

The major objective of this study was therefore to develop an integrated predictive and treatment-oriented framework in which ML-based water-quality assessment identifies contamination severity and GO-based treatment provides a potential route for pollutant and dye removal. Such integration may contribute to sustainable water-resource management and the development of low-cost nanomaterial-based wastewater treatment technologies.

## II. Material And Methods

### *2.1 Chemical parameters were analyzed using standard methods*

- pH – 6.5 to 8.5
- Alkalinity – 20 – 200mg/L ( as $caco_3$)
- Hardness – 100 -200 mg/L ( as $caco_3$)
- Chlorides – 200 – 600 mg/L
- Sulfates – 200 - 400 mg/L
- Nitrates – 50 - 100 mg/L ( as $NO_3$)
- Fluorides – 0.5 – 1.5 mg/L
- BOD( biological oxygen demand) – less than 5mg/L
- COD (Chemical oxygen demand) – less than 50mg/L

### *2.2 Machine Learning Model Development*

Multiple machine learning algorithms can be evaluated for prediction and classification of water quality. Suitable models include:

- Linear Regression
- Decision Tree
- Random Forest
- Support Vector Machine (SVM)
- k-Nearest Neighbour (k-NN)
- Gradient Boosting
- XGBoost

### *2.3 The degradation behavior*

The degradation behavior of three synthetic dyes—blue, violet, and maroon—was studied using UV photo-oxidation. Absorbance values were recorded at 2-minute intervals after treatment with hydrogen peroxide under UV light. The changes in absorbance are summarized below.

#### *1. Blue Dye*

The blue dye showed a sharp decrease in absorbance within the first 2 minutes, dropping from 0.34 to 0.18. However, subsequent readings remained relatively constant, indicating that most of the degradation occurred in the initial stage.

#### *2. Violet Dye*

For the violet dye, the absorbance decreased initially (from 0.81 to 0.44), indicating some level of degradation. However, an unexpected increase in absorbance was observed after 6 minutes, which may suggest re-aggregation of dye molecules, experimental inconsistency, or instrumental error. Further investigation is needed to clarify this anomaly.

#### *3. Maroon Dye*

The maroon dye showed an initial drop in absorbance from 1.32 to 0.99 in the first 2 minutes, but absorbance slightly increased and then stabilized. This could indicate a partial degradation followed by a plateau phase, suggesting that the dye may be more resistant to UV/$H_2O_2$ degradation compared to the blue and violet dyes

## III. Results And Discussion

The integrated analysis of water and dye samples demonstrates the usefulness of combining conventional laboratory analysis with computational and AI-assisted interpretation. The water-quality investigation identified several locations with elevated fluoride, nitrate, ammonia and COD. Among the analysed samples, Sample 5 was particularly important because of its high fluoride concentration of 15 mg/L and elevated COD of 340 mg/L.

The dye-degradation study demonstrated that the response of different dyes to UV/oxidative treatment was highly dependent on the dye system. Maroon dye showed an initial reduction followed by stabilization, while blue and violet dye datasets showed non-monotonic absorbance behaviour. These observations emphasize the importance of replicate experiments, appropriate blank correction and kinetic analysis before drawing definitive conclusions about degradation efficiency.

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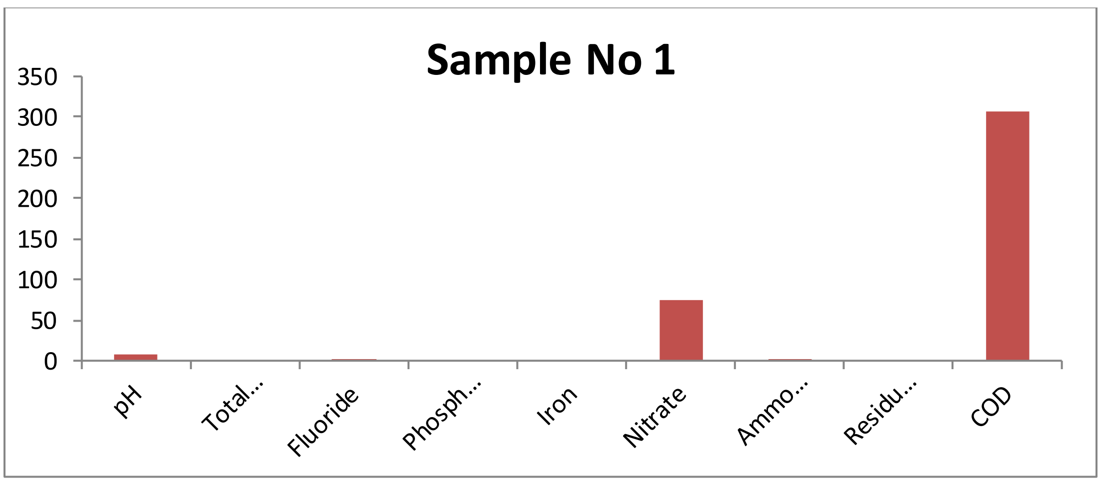
The AI-assisted WQI analysis provides an additional means of classifying environmental samples and identifying parameters that contribute to water-quality variation.

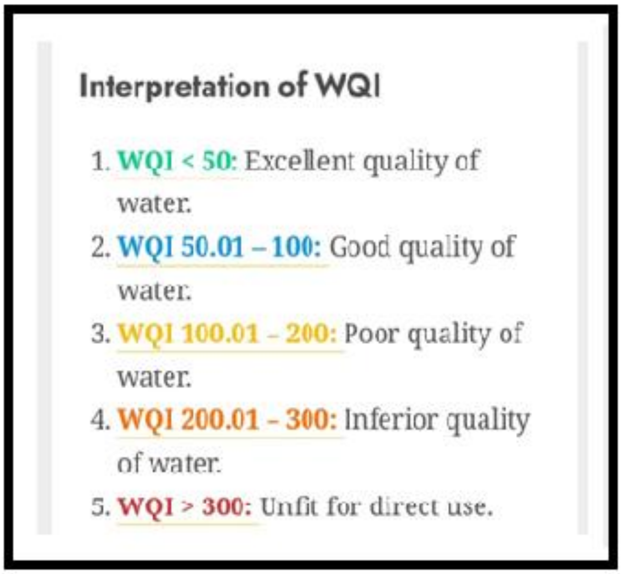
Nevertheless, AI predictions and WQI classifications should complement rather than replace standardized laboratory measurements.

**Table -3. 1 Water Quality parameters for sample 1:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 8.0 |
| Total Hardness | 60-120 | 0.0 |
| Fluoride | 1.4-6.0 | 1.5 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 0.5 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 306 |




*Sample no 1 -AI Tool 1*




*Interpretation of WQI*

*Sample no 1 shows WQI > 300, so this sample is unfit for direct use*

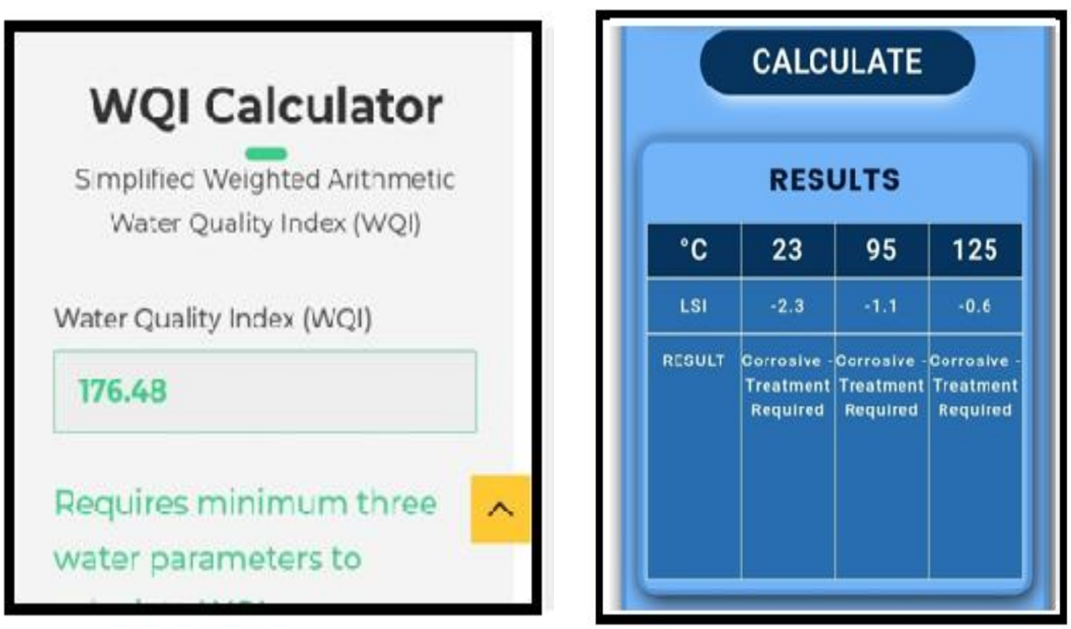



**Figure 3.2. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 1**

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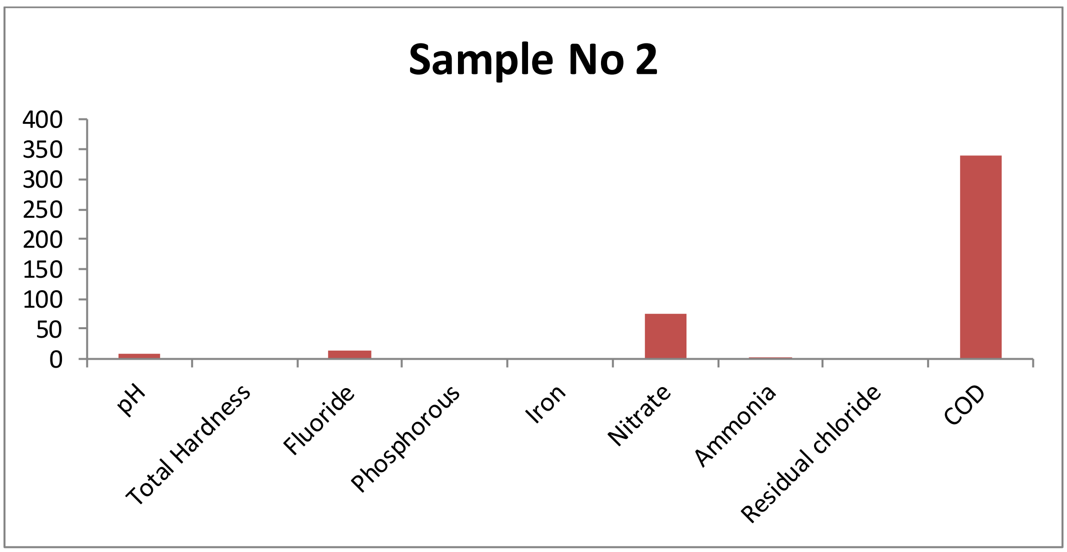
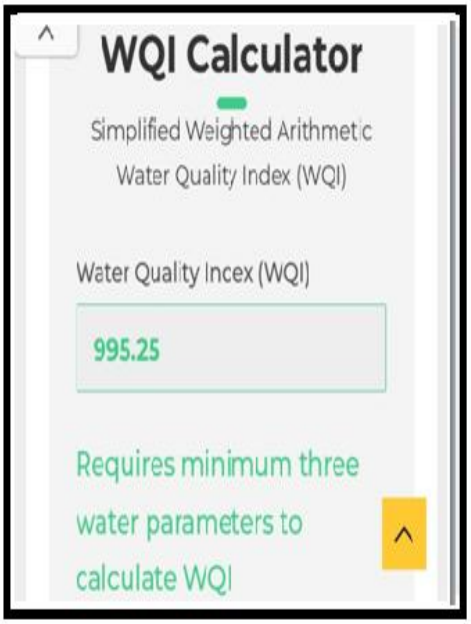
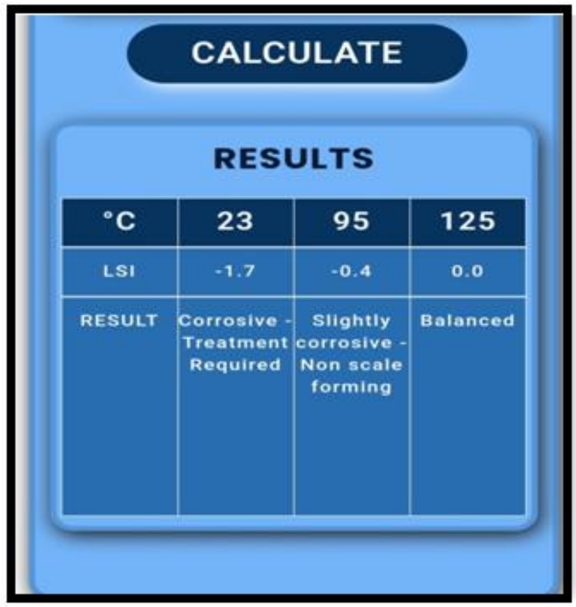
**Table -3. 2 Water Quality parameters for sample 2:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 9.0 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 1.0 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 15 |
| Ammonia | 0.5 | 0.5 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 312 |




*Sample no 2 AI Tool 1*




*Interpretation of WQI*

*Sample no 2 shows WQI > 300 , so this sample is unfit for direct use  AI Tool 2*

**Figure 2. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 2**

**Table – 3.3 Water Quality parameters for sample 3:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 8.5 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 15 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 0.5 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 340 |

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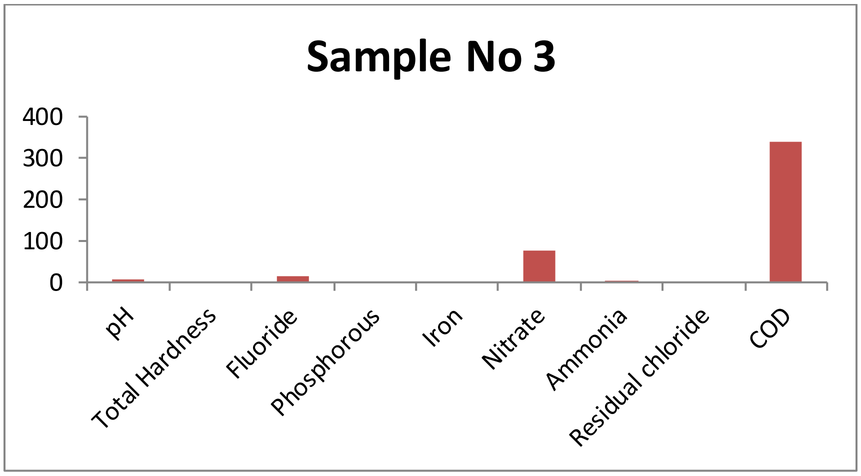


*AI Tool 1*

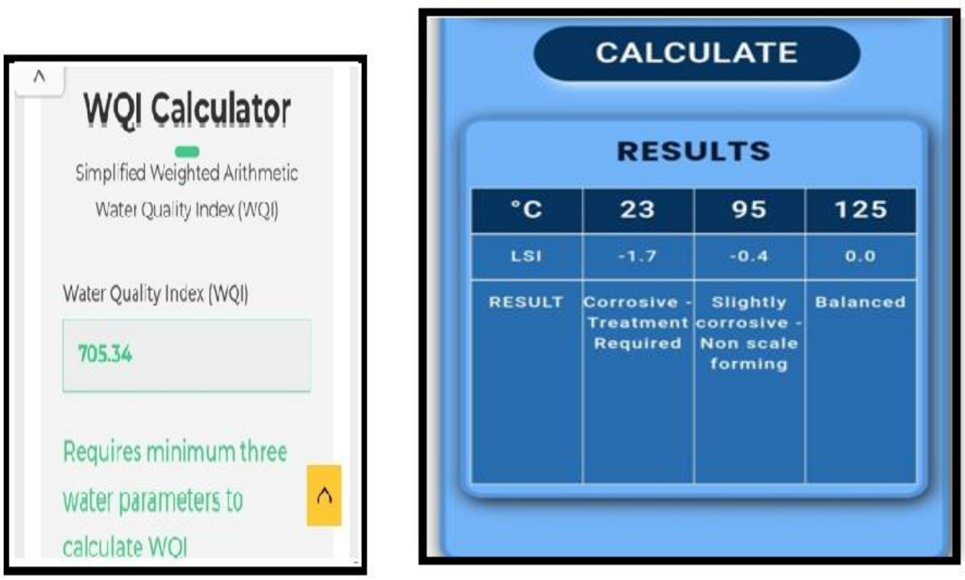


**Figure 3.3 Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 3 Interpretation of WQI**

*Sample no 3 shows WQI > 300, so this sample is unfit for direct use AI Tool 2*

**Table -3. 4 Water Quality parameters for sample 4:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 8.5 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 1.0 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 0.5 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 304 |

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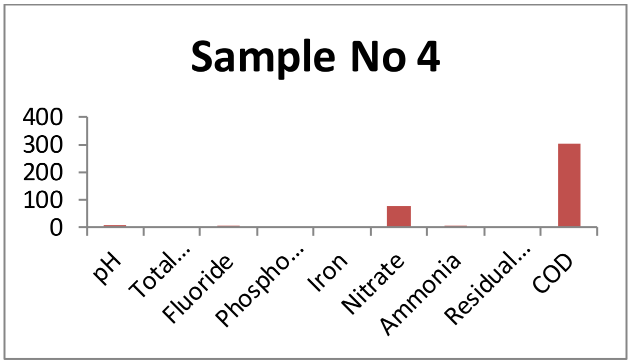
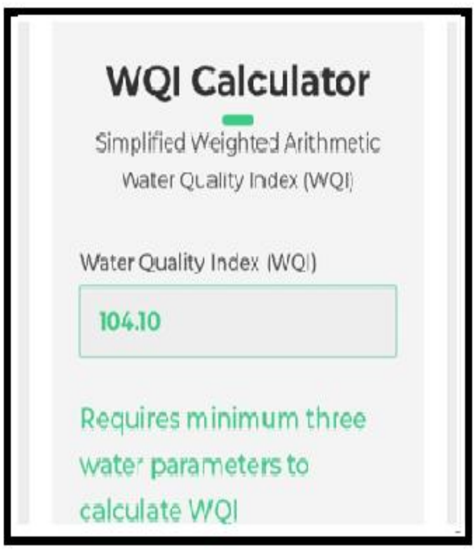



*AI Tool 1*



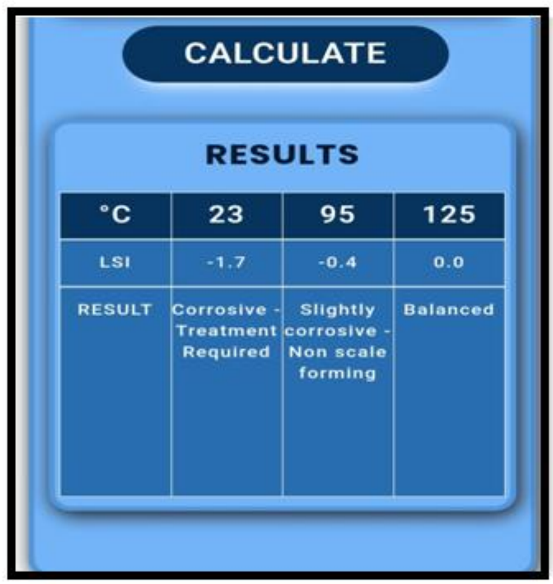
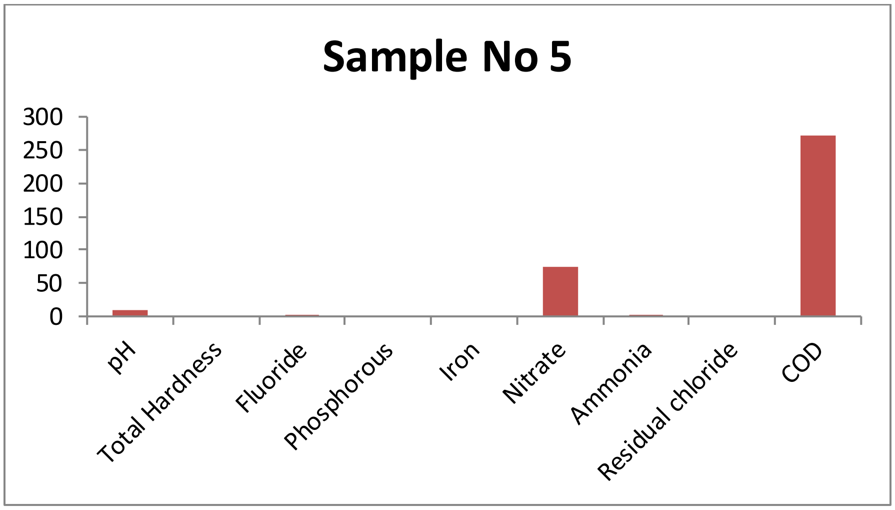




**Figure3. 4. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 4**

**Table – 3.5 Water Quality parameters for sample 5:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 6.5 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 0.5 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.3 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 0.5 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 292 |




*Sample no 5*

*AI Tool 1*

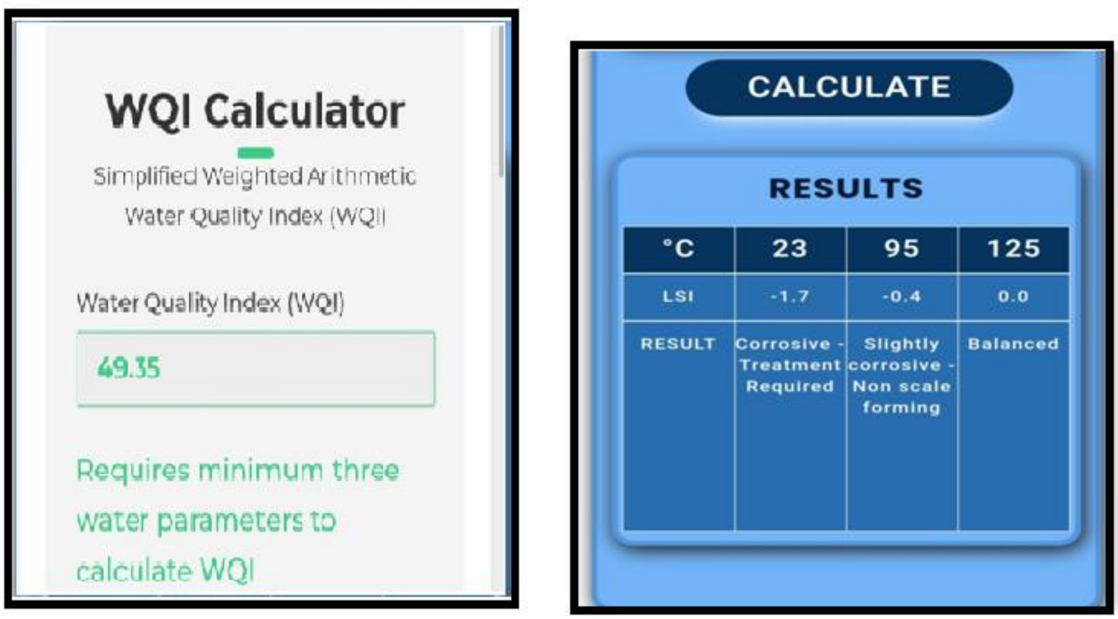
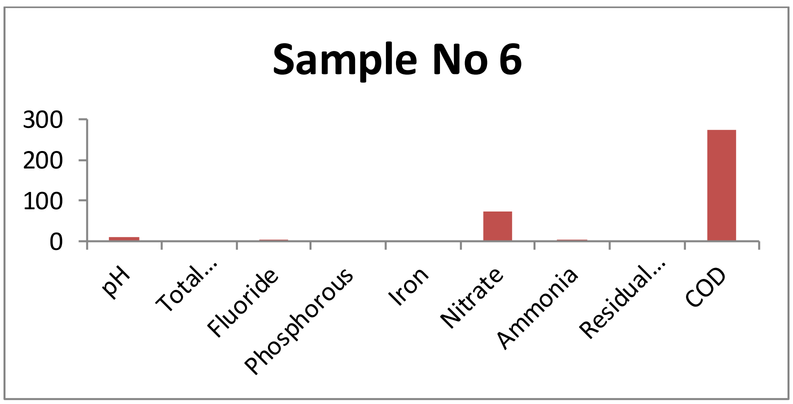



**Figure 3. 5. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 5**

**Table - 6 Water Quality parameters for sample 6:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 6.5 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 0.5 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 1.0 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 306 |



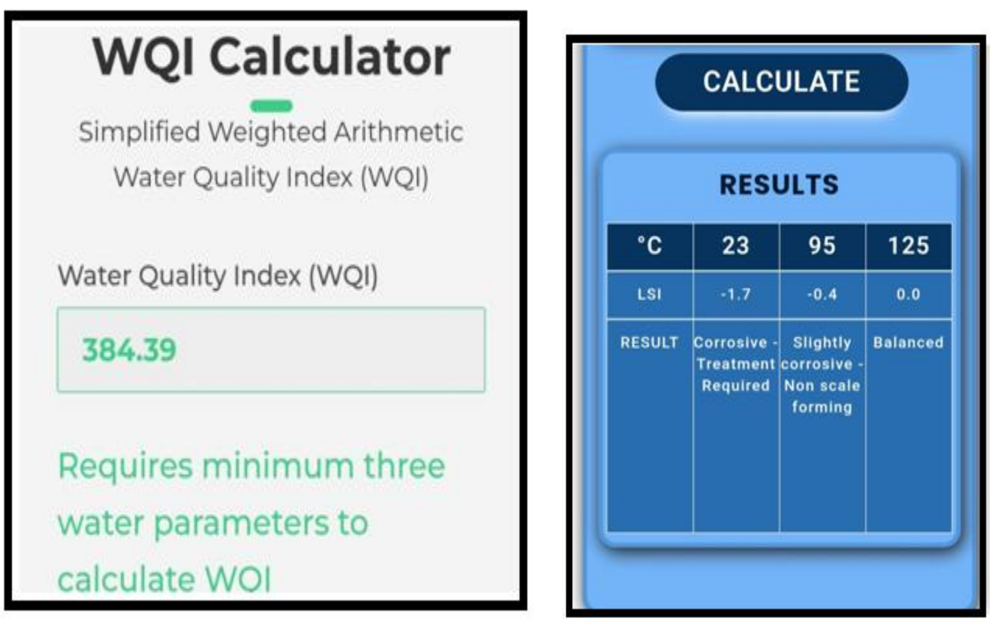




**Figure 6. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 6**

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Table -3. 7 Water Quality parameters for sample 7:

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 6.5 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 1.0 |
| Phosphorous | 0.005-0.05 | 0.5 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 75 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 274 |

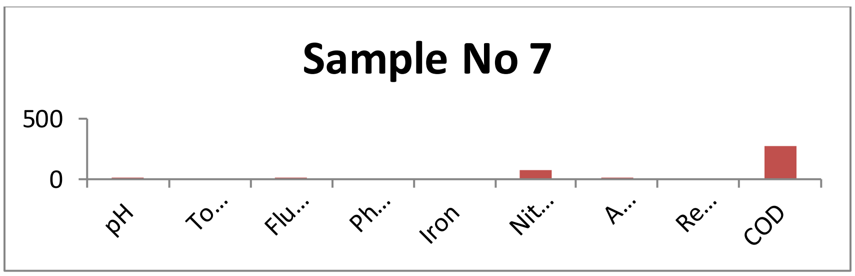
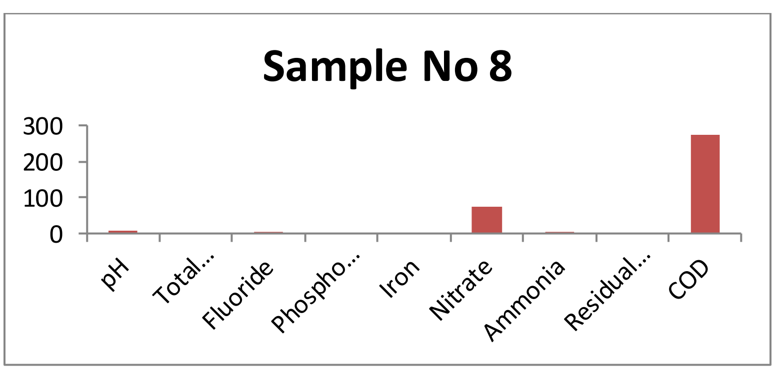



Figure 7. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 7

Table – 3.8 Water Quality parameters for sample 8:

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 9.0 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 1.0 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 1.0 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 272 |



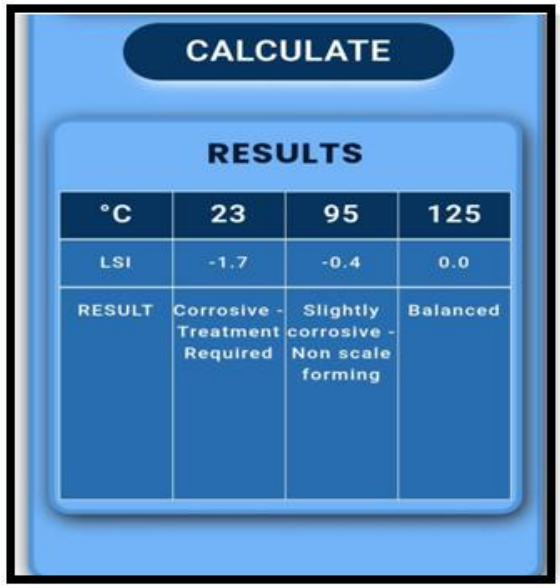
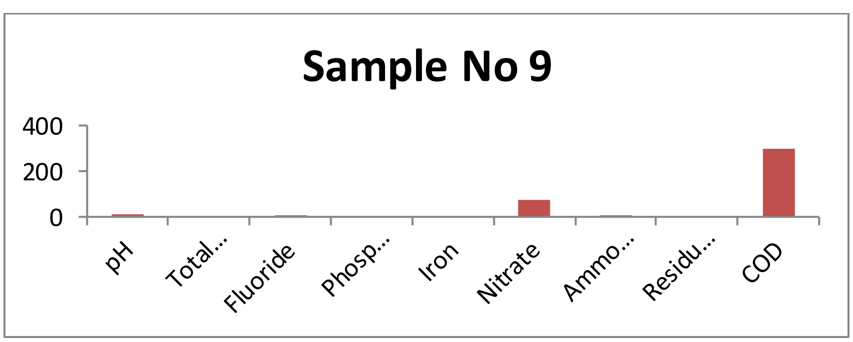




**Figure 3.8. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 8**

**Table -3. 9 Water Quality parameters for sample 9:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 8.0 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 1.0 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 1.0 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 296 |



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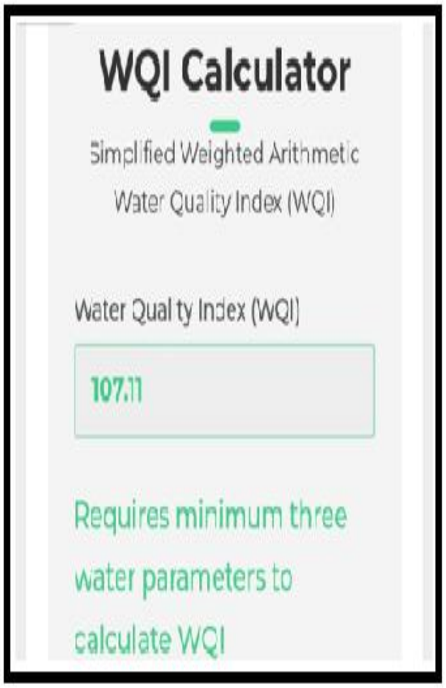



**Figure 3.9. Machine Learning-Based Computation of the Water Quality Index (WQI) for Sample 9**

**Table – 3.10 Water Quality parameters for sample 10:**

| Parameter | Reference (mg/L) | Testing value (mg/L) |
|---|---|---|
| pH | 6.5-8.5 | 9.0 |
| Total Hardness | 10-500 | 0.0 |
| Fluoride | 1.4-6.0 | 1.0 |
| Phosphorous | 0.005-0.05 | 0.0 |
| Iron | 0.3 | 0.0 |
| Nitrate | 10 | 75 |
| Ammonia | 0.5 | 2.0 |
| Residual chloride | 0.2-0.5 | 0.0 |
| COD | 200-300 | 250 |

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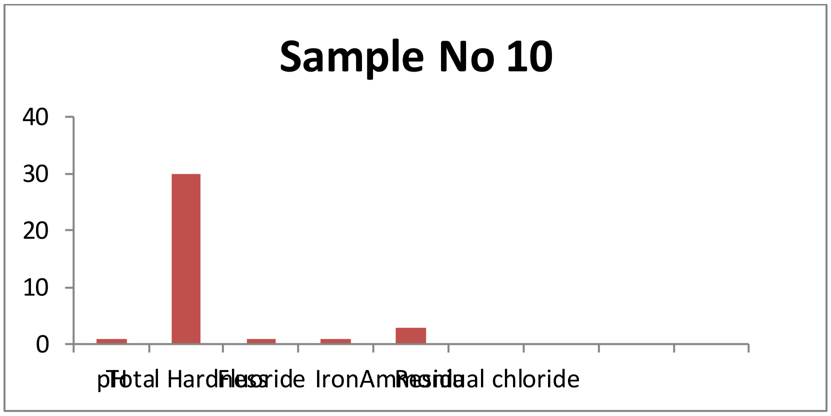


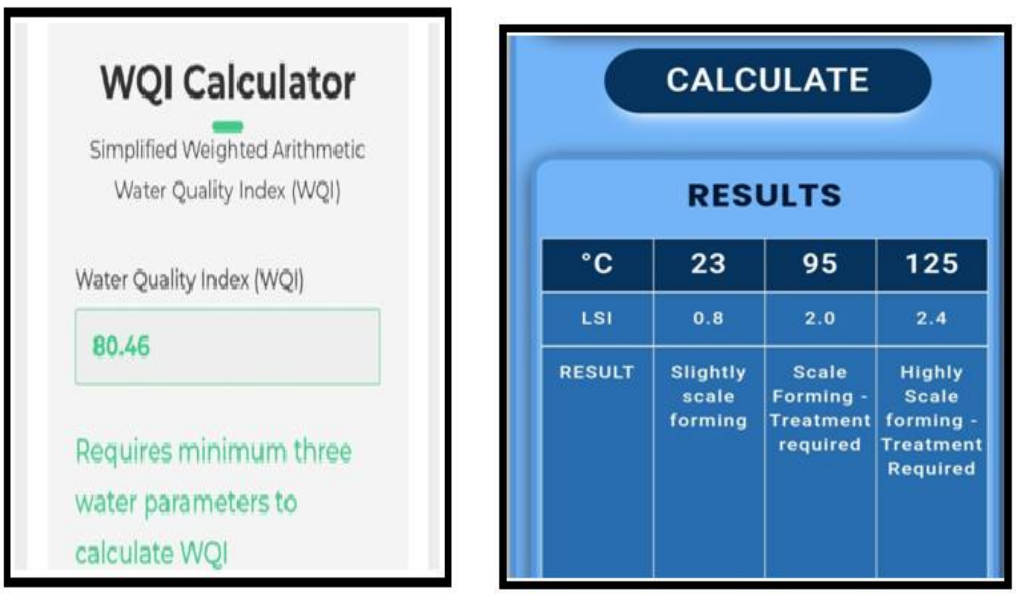


**Figure 3.10. Machine Learning-Based Computation of the (WQI) for Sample 10**

This study involves the application of machine learning tools like AI tools which was employed to classify water samples as potable or non potable .The study implemented an artificial intelligence framework for water quality assessment, utilising ensemble learning methods to process multi-parameters water quality data. In this study, the three AI tools were employed

## IV. The Degradation Behavior Of Three Synthetic Dyes

Here are the individual graphs for each dye:

1. *Blue Dye* – shows rapid initial degradation and then stabilization

2. *Violet Dye* – shows irregular pattern with re-increase in absorbance.

3. *Maroon Dye* – gradual decrease and then stabilization, indicating resistance to degradation

*4.1 Graphical representation*

*Blue colour dye (Max value 450)*

| Timing (Minutes) | Absorption |
|---|---|
| 0 | 0.34 |
| 2 | 1.18 |
| 4 | 1.19 |
| 6 | 1.19 |
| 8 | 1.19 |
| 10 | 1.19 |

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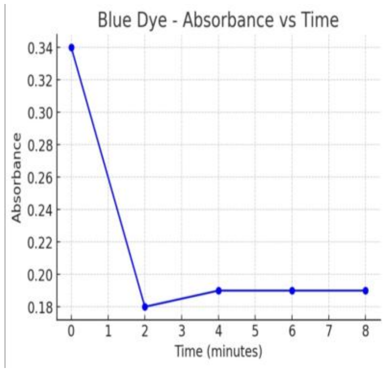


**Figure 1: Blue Dye – Absorbance vs. Time**

The graph shows a rapid decrease in absorbance during the first 2 minutes, indicating significant degradation under UV/$H_2O_2$ treatment. The absorbance values stabilize after 2 minutes, suggesting most of the degradation occurred initially.

*Violet colour dye (Max value 400)*

| Timing (Minutes) | Absorption |
|---|---|
| 0 | 0.81 |
| 2 | 1.48 |
| 4 | 1.44 |
| 6 | 0.81 |
| 8 | 0.81 |
| 10 | 0.81 |

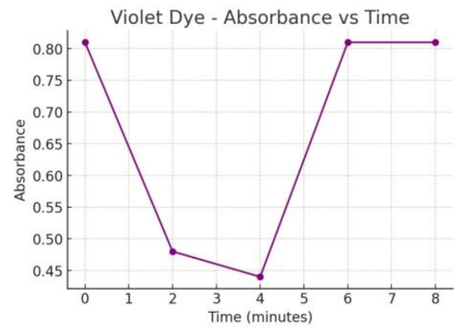


**Figure 4.2: Violet Dye – Absorbance vs. Time**

This graph depicts an initial reduction in absorbance, followed by an unexpected rise. This could be due to reaggregation, instrumental error, or reversible reactions occurring during UV exposure

*Maroon colour dye (Max value 680)*

| Timing (Minutes) | Absorption |
|---|---|
| 0 | 1.32 |
| 2 | 0.99 |
| 4 | 1.06 |
| 6 | 1.06 |
| 8 | 1.05 |
| 10 | 1.05 |


**Figure 4.3: Maroon Dye – Absorbance vs. Time**

The maroon dye shows a gradual decline in absorbance with a minor increase, eventually stabilizing.

This indicates a relatively resistant nature to UV/$H_2O_2$ degradation, possibly due to a more stable molecular structure.

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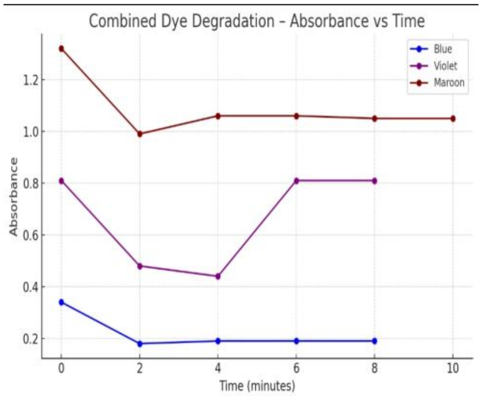


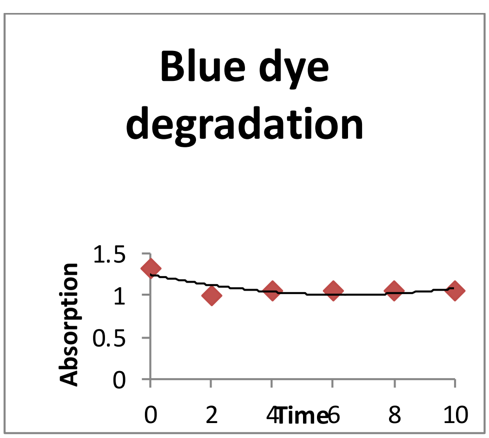

**Figure 4: Combined Dye Degradation – Absorbance vs. Time**

This graph compares the absorbance changes of blue, violet, and maroon dyes over time under UV/$H_2O_2$ treatment. The blue dye shows the fastest degradation, the violet dye displays irregular behavior, and the maroon dye degrades more slowly and stabilizes, indicating resistance.

*Dye degradation (Oxidation agent GO/$H_2O_2$)*

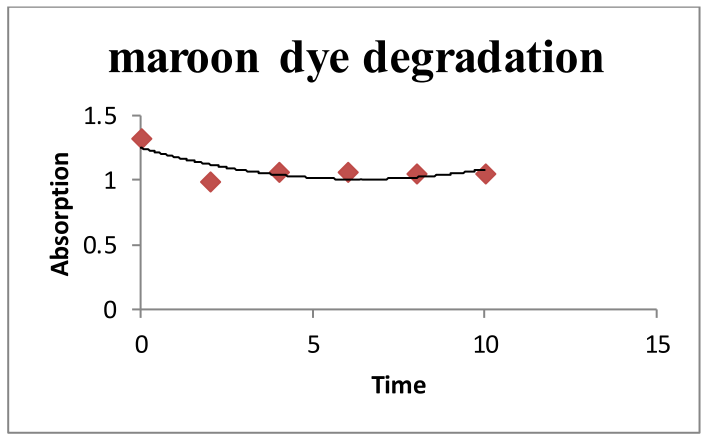
*Blue colour dye (Max value 450)*

| Timing (Minutes) | Absorption |
|---|---|
| 0 | 0.34 |
| 2 | 1.18 |
| 4 | 1.19 |
| 6 | 1.19 |
| 8 | 1.19 |
| 10 | 1.19 |



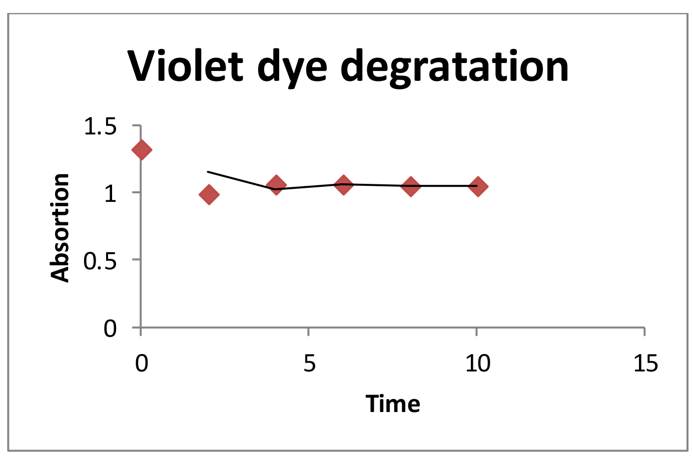

*Maroon colour dye (Max value 680)*

| Timing (Minutes) | Absorption |
|---|---|
| 0 | 1.32 |
| 2 | 0.99 |
| 4 | 1.06 |
| 6 | 1.06 |
| 8 | 1.05 |
| 10 | 1.05 |




*Violet colour dye (Max value 400)*

| Timing (Minutes) | Absorption |
|---|---|
| 0 | 0.81 |
| 2 | 1.48 |
| 4 | 1.44 |
| 6 | 0.81 |
| 8 | 0.81 |
| 10 | 0.81 |



## V. Water Quality Index And AI-Based Interpretation

An artificial-intelligence-assisted approach was employed to support the classification of water samples based on their overall water quality. Multiple AI tools were used to process the measured physicochemical parameters and assist in identifying samples requiring attention.

Sample 8 was interpreted as having a WQI in the range of approximately 100.1–200 and was therefore classified as having poor water quality. In contrast, Sample 9 was interpreted as having a WQI below 50 and was classified as excellent according to the adopted WQI classification. Sample 10 showed a WQI greater than 300 and was classified as unfit for direct use.

The AI-assisted analysis demonstrates the usefulness of computational tools for rapid classification of water-quality data. However, WQI values are highly dependent on the parameters selected, their weighting factors, sampling frequency, geographical location and the particular WQI methodology employed. Consequently, AI-based classification should be considered a decision-support approach and should be validated against standard laboratory methods and applicable drinking-water standards.The analysis also highlights the importance of identifying the key parameters responsible for water-quality deterioration. Parameters such as fluoride, nitrate, ammonia, COD and pH contributed substantially to the observed differences between sampling locations. The results indicate that contaminated samples require suitable treatment before domestic or drinking-water use.

The degradation behaviour of blue, violet and maroon synthetic dyes was investigated under UV/photo-oxidative conditions. Changes in absorbance were monitored at two-minute intervals. Absorbance was used as an indicator of the concentration of the coloured species remaining in solution.

## VI. Dye Degradation Using Graphene Oxide/ $H_2O_2$ As Oxidation/Catalytic System

The degradation experiments were also examined using GO/HP based treatment. The blue, maroon and violet dye solutions were characterized after treatment using selected water-quality parameters.For the blue dye sample, the measured pH was 1.0, total hardness was 30 mg/L, fluoride was 1.5 mg/L, iron was 0.3 mg/L, ammonia was 1.0 mg/L and residual chloride was 0.2 mg/L. The very low pH indicates strongly acidic conditions and should be carefully controlled before considering any treated solution for environmental discharge or reuse.

The post-treatment results indicate that dye degradation alone does not necessarily mean that the treated water is suitable for discharge or reuse. The final pH and other water-quality parameters must also be evaluated. In particular, the strongly acidic pH values observed after treatment require neutralization and further treatment before environmental application.

The calculation should be performed using corrected absorbance values at the appropriate wavelength ($\lambda$max).

The present investigation evaluated the quality of water and soil samples collected from selected locations around Madurai and examined the degradation behaviour of selected synthetic dyes using oxidative treatment.

## VII. Summary And Conclusion

Graphene oxide (GO) demonstrated promising potential as a multifunctional material for water purification, hardness reduction, and dye degradation. The oxygen-containing functional groups present on the GO surface provide abundant active sites for interaction with dissolved ions and organic dye molecules. The experimental results indicate that GO can effectively contribute to the removal of hardness-causing ions and the degradation/removal of coloured pollutants from contaminated water.

The dye-degradation study further demonstrated that GO-based treatment can reduce dye concentration under suitable oxidative/photocatalytic conditions. The degradation efficiency is influenced by factors such as GO dosage, initial dye concentration, pH, contact time, oxidant concentration and irradiation conditions. Optimization of these parameters can significantly improve the overall treatment efficiency.

The combined ability of GO to address inorganic contaminants responsible for water hardness and organic dye pollutants makes it a promising candidate for advanced wastewater treatment. Therefore, GO-based materials can provide a potentially effective and sustainable approach for improving water quality. Further studies should focus on GO–MXene or GO-based composite membranes, regeneration and reuse of the material, treatment of real wastewater, toxicity assessment, and scale-up for practical water-purification applications.

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