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Research paper

Wastewater Treatment with Carbon-Based Nanomaterials Enhanced by Real-Time Machine Learning Based Monitoring

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Abstract

Intelligent adaptive control is required for the effective treatment of wastewater using carbon-based nanomaterials due to the dynamic and complex nature of pollutant removal mechanisms. This study improves anomaly detection and predictive monitoring in treatment systems that use carbon derivatives such as graphene oxide (GO) and graphite activated carbon (AC) by applying machine learning (ML) techniques. A treatment facility in Maharashtra supplied operational data from 2023 to 2025, including 18,250 daily records by combining real-time sensor data with laboratory analysis during that time. The zeta potential of the heavy metals BOD and COD, the dosage of the nanomaterials, the pH, contact time, and the turbidity were all significant factors. Measurement tools like ICP-OES, UV-VIS spectrophotometers, and SCADA-GIS interface turbidity meters were used to guarantee high temporal and spatial granularity. Temporal patterns and operational anomalies were recorded using machine learning models called Random Forest Regressor, Autoencoders, and Temporal Convolutional Networks (TCNs). Autoencoders identified deviations such as membrane fouling. Random Forests identified significant factors influencing treatment efficacy, and TCNs effectively modeled trends in pollutant concentrations. An ensemble modeling approach was applied to improve prediction robustness. MAPE, NRMSE, and precision-recall metrics were used to assess the model. The results demonstrated increased operational reliability, more accurate fault detection, and more informed dosage selections. Ultimately, complementary techniques like optical microscopy and scanning electron microscopy (SEM) were used to describe these nanomaterials in order to confirm their surface morphology, elemental composition, and functional integrity. Thus, the machine learning-integrated framework promotes data-driven, environmentally friendly wastewater treatment using cutting-edge carbon nanomaterials.

Keywords: *Carbon Nanomaterials; Wastewater Treatment; Anomaly Detection; Machine Learning; TCN; Random Forest.*

1. Introduction

Nanomaterials are now very promising agents in wastewater treatment systems because of their exceptional physicochemical properties, such as high surface area reactivity and tunable surface functionalities. Nanomaterials' unique properties allow them to interact at the molecular level with various pollutants, increasing the effectiveness of their removal of contaminants like organic compounds, heavy metals, dyes, and pathogens. Materials like carbon nanotubes, graphene oxide, metal nanoparticles (like iron, titanium dioxide, and silver), and nanocomposites are being extensively studied and utilized for their adsorption, photocatalytic, and antimicrobial properties. For instance, silver nanoparticles have strong antibacterial qualities that aid in wastewater disinfection, and titanium dioxide nanoparticles can photocatalyze the breakdown of organic pollutants when exposed to UV light. Additionally, nanomaterials can be incorporated into coatings or membranes to improve filtration efficiency, reduce fouling, and prolong the life of treatment systems. Waterborne solids and liquids that are dumped into sewers as waste are referred to as wastewater. Organic materials that are dissolved and suspended in wastewater can break down biologically.

Wastewater is treated by removing some of the particles and utilizing decomposition to turn highly complex organic solids into more stable ones. In the first and secondary stages of wastewater treatment, most of the suspended solids (SS) and biological oxygen demand (BOD) are eliminated. Wastewater treatment facilities have added additional treatment procedures to further remove organic solids, nutrients and

hazardous contaminants, even though this level of treatment has proven insufficient to produce recycled water for use in homes and businesses.

A recent analysis of carbon-based materials has shown that artificial wetlands are an effective wastewater treatment technique. Compared to traditional treatment facilities, constructed wetlands are less expensive and simpler to maintain. They have a wide range of possible uses, particularly in developing nations' tiny rural areas. [1] By examining the outcomes of research programs aimed at implementing the technology in developing nations, the researcher has further investigated the possibilities of artificial wetlands for wastewater treatment and reuse in these nations. [2]. Because of their large surface area, chemical stability, and structural tunability, carbon nanomaterials have become popular options for a variety of remediation applications, including the adsorption of organic chemicals, dyes, and heavy metals [3].

Initiatives to reduce wastewater and recycle water can be combined with the ongoing research being done on advanced wastewater treatment technologies. Membrane technology has developed into a respectable separation technique that requires no additional chemicals and operates with very little energy consumption and well-organized process conduction. [4]. Furthermore, lowering the amount of biomass produced during aerobic metabolism must encourage the conversion of organic contaminants into respiratory products while also raising the need for aeration. Promoting extra metabolism of absorbed organic carbon will result in the release of more respiration products and a decrease in the total amount of biomass produced. Reduced biomass generation in the environment might be the outcome of purposeful process operations and appropriate physical conditions. [5]. Based on economic prospects, employing machine learning approaches, wastewater reuse lowers the cost of wastewater disposal and freshwater supply.

Reusing a significant volume of wastewater usually entails treating or regenerating the available wastewater to satisfy strict water quality standards. On the other hand, when pollutant removal efficiency increases, the processing cost of reusing wastewater increases exponentially [6]. They have shown how crucial it is to strike a balance between these conflicting cost variables, which depend on the concentration of contaminants after regeneration or treatment. With either wastewater regeneration reuse or wastewater treatment reuse, the overall cost of the wastewater reuse system may be reduced using this cost optimization process [7]. Among the notable benefits of anaerobic methods, particularly for carbon nanomaterials, are high organic loading rates and minimal sludge generation [8].

One of the main factors driving the growing use of anaerobic technologies is energy production. In addition to producing positive net energy, this technology also produces biogas, which may take the place of fossil fuels and so directly contribute to the reduction of greenhouse gas emissions [9].

Furthermore, a variety of nanomaterial classes have been discovered in a significant amount of biomass (50%) is retained in the interstitial spaces of the filters rather than being firmly affixed to the support medium. The early designs of minimal voidage, rock-packed reactors have mostly been superseded by systems that use synthetic packing materials to allow the buildup of non-attached biomass without blocking the bed. [10].

A waste stream was directed uphill through a bed of randomly arranged quartzite stones as a matrix for cell immobilization in an early version of the fixed-bed anaerobic process [11]. The short hydraulic retention durations and high organic loading rates attained in this first "anaerobic filter" were made possible by the development of biofilm on the quartzite stones' surface [12]. An important factor in improving the wastewater treatment plant's performance is modeling it with activated sludge. The amount of data accessible for calibration, model identification, and verification is still severely limited by the presence of missing values and outliers in datasets. Even though there is typically little data available, gaps and outliers in the data must be replaced [13]. The pre-treatment of waste activated sludge employed the Newton method for the network's hydraulic analysis and the Genetic algorithm optimization methodology to choose the best network design in pipe network optimization [14]. These advancements assessed the latest Ant-Colony-based algorithm and its use in a system with many reservoirs. As the number of choice factors rises, more computing time is needed, and less-than-ideal solutions are produced. Therefore, unless specific changes are taken into consideration, the Ant-Colony-based algorithm would not be able to tackle complicated water resource problems. [15]. Additionally, the PSO technique's vast population variety allowed agricultural waste-derived nanoparticles to apply it to other industrially relevant challenges in the water industry, finding optimal or nearly optimal solutions much more quickly and with far less computing work. [16].

A novel method for training the Adaptive Network Based Fuzzy Inference System (ANFIS) was presented with the growing popularity of green and sustainable nanomaterials. To train all the parameters of the ANFIS structure, they used Particle Swarm Optimization (PSO), one of the swarm intelligence branches, with certain changes [17]. These changes are inspired by natural evolution. Finally, this technique was used to identify non-linear dynamical systems, and the results of comparing it to basic PSO were rather good. Using an objective optimization model that was developed and resolved by a particle swarm optimization method, this maximized the production of biogas. By identifying the settings of controllable variables, the author of this work examined how the PSO algorithm calculates the optimal fitness of biogas production [18].

For assessing the effluent COD of an anaerobic wastewater treatment plant under unstable conditions using carbon nanomaterials, a neural-fuzzy model based on ANFIS was previously proposed. However, ANFIS often fails to handle high-dimensional inputs and is not robust in dynamic temporal contexts. By combining Random Forests (RF) for feature-level interpretability and Temporal Convolutional Networks (TCNs) for capturing long-range temporal dependencies, our stacking ensemble circumvents these limitations in contrast to ANFIS. This enhances the explainability, scalability, and accuracy of real-time COD predictions [19]. To wrap up, the author looked at how well the ANN could reproduce the relationships between different water quality indicators. The best ANN model and modeling process are chosen for the carbon nanomaterials after a review of various ANN architectures, inputs, and training options. The predictive powers of autocorrelated residuals and linear regression models were examined and contrasted with those of the ANN. They also concluded that ANN models outperform linear regression models in terms of accuracy [20].

Implementing advanced treatment and prediction systems is hampered by nanomaterial deterioration and machine learning (ML) scalability, especially in large-scale wastewater facilities. For instance, even though graphene oxide (GO) is effective at eliminating pollutants, its adsorption efficiency gradually declines as a result of structural deterioration and fouling. The accumulation of inorganic and organic materials on the GO surface causes fouling, which harms the active sites. ML models, which enable performance optimization and predictive maintenance, mitigate this. They also make it possible to detect performance drops early and implement adaptive control strategies that alter system parameters in real time to maintain treatment efficacy and extend nanomaterial lifespan.

2. Materials and methods

A systematic approach to optimizing and detecting anomalies in wastewater treatment systems upgraded with carbon-based nanomaterials is described in the materials and methods section that follows. Subsections on problem context, data collection plans, nanomaterials

characterization, measurement tools, and parameter ranges highlight the study's most important findings. It also offers details on the analytical techniques used on the processed samples and the recommended machine learning techniques, along with a theoretical underpinning for machine learning. The approach ends with a proposal for multi-model integration, and performance metrics are used to assess the developed system's resilience and effectiveness.

2.1. Problem description

The limitations of this study are

1) Wastewater treatment using carbon-based nanomaterials, though promising in terms of high adsorption efficiency and selectivity, is hindered by inherent operational uncertainties. These arise due to the fluctuating nature of influent characteristics such as pH, biochemical oxygen demand (BOD), chemical oxygen demand (COD), and the variable presence of heavy metals.
2) Traditional static models are incapable of capturing these nonlinear and time-varying dependencies.
3) Moreover, the long-term sustainability of the treatment process is affected by delayed recognition of nanomaterial degradation, fouling, or under-/over-dosing. Consequently, the lack of intelligent monitoring tools often leads to inefficiencies, higher operational costs, and regulatory non-compliance.
4) This research addresses these limitations by integrating advanced machine learning models into the treatment pipeline to facilitate dynamic process adaptation and intelligent fault prediction.

2.2. Data collection

Operational data was collected over two years (2023–2025) from a mid-scale wastewater treatment facility located in Maharashtra, India. The system integrates both conventional and nanomaterial-assisted treatment modules. A total of 18,250 daily records were acquired, capturing temporal variations across multiple treatment stages, which is shown in Table 1. Real-time data from Supervisory Control and Data Acquisition (SCADA) systems was synchronized with laboratory-verified analytical measurements for comprehensive process representation.

Table 1: Data Collection Summary

Data Source	Instrument/Technique	Frequency	Parameter Types
SCADA System	Integrated GIS-SCADA	Every 15 minutes	Flow rate, pressure, system logs
UV-VIS Spectrophotometer	Online (automated)	Daily	BOD, COD
Turbidity Sensors	Online (nephelometric)	Hourly	Turbidity
ICP-OES (Agilent 5110)	Laboratory	Biweekly	Heavy metals (Pb, Cd, Cr, Hg)
Zeta Potential Analyzer (Zetasizer Nano ZS)	Laboratory	Weekly	Surface charge, nanomaterial stability
Manual Sampling and Lab Analysis	Gravimetric/Volumetric	Daily	pH, contact time, nanomaterial concentration

2.3. Materials

Graphite and activated carbon, which were acquired from Sigma-Aldrich and Cabot Corporation, were utilized as raw materials in the investigation. Additionally, graphene oxide was acquired from Sigma-Aldrich. A modified Hummer's technique was used in a lab to create graphene oxide (GO). GO water dispersion was used to create lyophilized GO forms and air-dried materials. Water-dispersed GO, designated GO-T1 and GO-T2, was used in the experiments three and thirty-six weeks following the synthesis period. All GO forms were kept at room temperature in airtight jars which as shown in Figure 1.

Fig. 1: An Overview of the Carbon Materials Under Investigation Includes Graphite (A), Activated Carbon Norit SA Super (B), Commercial Graphene Oxide (GO_C) (C), Graphene Oxide (GO_T1; D; E), Graphene Oxide (GO_AD) (F) After Air Drying, and Graphene Oxide (GO_L) After Lyophilization.

2.4. Data measurement

The provided Figure 2 illustrates a four-layer generic SCADA (Supervisory Control and Data Acquisition) architecture. The Field layer at the bottom consists of sensors and actuators that interact directly with the physical process, connected via electrical wiring and a fieldbus. The Local control layer above it utilizes PLCs (Programmable Logic Controllers), RTUs (Remote Terminal Units), and HMIs (Human-Machine Interfaces) to manage and automate local operations, communicating with field devices often through protocols like PROFINET. These local control elements are connected to the higher layers through wired or wireless connectivity. The Communication layer facilitates data exchange using various technologies such as GPRS, Internet, Radio, Satellite, OPC, and VPN, enabling communication between the local control and supervisory levels. Finally, the Supervisory layer at the top employs SCADA systems, databases, and HMIs (represented by monitors) to monitor, control, and manage the entire system remotely, often connecting to external networks via a modem.

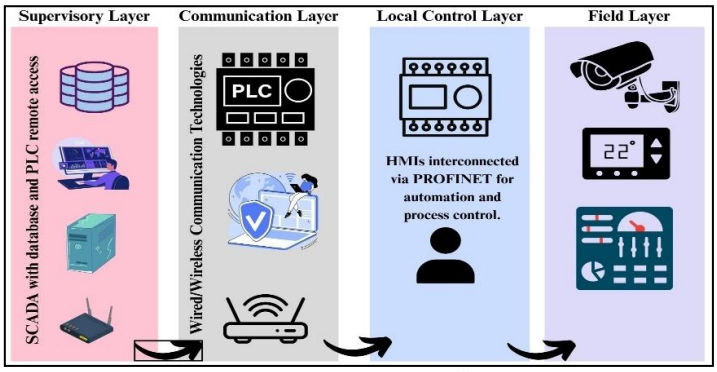

Fig. 2: Four-Layer SCADA Architecture.

2.5. Parameter distribution

The parameter ranges in Table 2 were carefully selected to reflect realistic wastewater characteristics and optimize adsorption performance using carbon-based nanomaterials. The pH range of 5.8–9.2 captures typical variability in industrial effluents, influencing ionization and surface charge interactions. BOD (20–650 mg/L) and COD (60–1200 mg/L) encompass low to high organic and oxidizable pollutant loads, simulating both domestic and industrial wastewater conditions. Turbidity (2–380 NTU) addresses a broad range of suspended solids, affecting mass transfer during adsorption. The lead concentration range (0.01–0.9 mg/L) represents toxic metal levels commonly found in industrial discharges. Zeta potential (–45 to +10 mV) provides insight into colloidal stability and electrostatic interactions. Contact time (5–180 minutes) allows for kinetic analysis from rapid adsorption to equilibrium, while the nanomaterial dose range (10–200 mg/L) evaluates adsorption efficiency across low to high material loading. These ranges ensure experimental relevance, robustness, and reproducibility.

Table 2: Key Parameters and Their Physical-Chemical Properties

Parameter	Range	Units	Role	Type
pH	5.8 – 9.2	-	Adsorption kinetics	Chemical
BOD	20 – 650	mg/L	Organic load indicator	Chemical
COD	60 – 1200	mg/L	Oxidizable pollutants	Chemical
Turbidity	2 – 380	NTU	Solids concentration	Physical
Heavy Metals (Pb)	0.01 – 0.9	mg/L	Toxic metal contamination	Chemical
Zeta Potential	–45 to +10	mV	Surface charge interaction	Physical
Contact Time	5 – 180	minutes	Adsorption efficiency	Physical
Nanomaterial Dose	10 – 200	mg/L	Adsorption capacity	Operational

2.6. Sample analysis

To validate real-time sensor data and investigate the physicochemical changes during treatment, samples were collected at three critical points in the system: the influent (raw wastewater), the mid-treatment stage (post-primary and secondary treatment), and the effluent (post-nanomaterial contact). Sample analysis adhered to the Standard Methods for the Examination of Water and Wastewater (APHA, 23rd Edition), ensuring methodological consistency and traceability. BOD and COD were measured using closed reflux colorimetric methods with absorbance read via UV-VIS spectrophotometry. Heavy metal content was assessed following acid digestion using nitric and hydrochloric acid mixtures, and quantified using ICP-OES (Agilent 5110 series). Turbidity was measured using nephelometric techniques, while pH was determined using a microprocessor-based bench-top meter (Hanna HI5221). Nanomaterial residues were isolated post-treatment through centrifugation and characterized using FTIR and SEM to monitor any morphological or chemical changes, such as pore structure collapse or surface fouling.

2.7. Proposed techniques

Figure 3 illustrates the application of machine learning in wastewater treatment, integrating a physical wastewater treatment process with a neural network model. The lower section depicts a typical wastewater treatment plant, including a biological reactor and a secondary settler tank, where sensors (AODJ-QX6530, WTW oxi/340i, CHM-300, 7110 MTF-FG, pH700) measure key parameters like ORP, SO2, SPO4, TSS, and PH from the influent and different stages. These raw sensor data are fed into the machine learning system (upper section), where they undergo preprocessing and normalization to create a training database. This database is then used to train a neural network, which takes the five measured parameters (x1 to x5 representing SPO4, ORP, SO2, TSS, and PH, respectively) as inputs to predict the output SNH, likely representing the treated water quality or a specific nitrogen compound concentration.

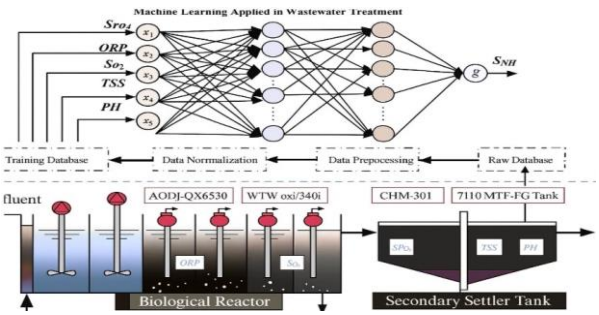

Fig. 3: Integrated Machine Learning Framework for Wastewater Treatment Monitoring and Prediction.

By leveraging ensemble learning, deep learning, and unsupervised learning strategies, the proposed approach is capable of modeling both continuous treatment performance (e.g., pollutant removal) and rare anomalous events (e.g., fouling or dosing failure). The techniques are further strengthened with optimization strategies and robust evaluation metrics to ensure reliability in real-time scenarios. Eight foundational equations form the computational basis of the proposed framework, representing both the functional operation of each model and the performance evaluation metrics used for its validation.

The mathematical models of this work are expressed from equations 1 to 8:

Random Forest is a powerful ensemble learning algorithm that is based on the idea of constructing a multitude of decision trees at training time. Every tree ht(x) ∈ H in the ensemble serves as a weak learner based on a random sample of data and features. The final prediction is obtained by averaging over all the predictions of the T trees.

$$\hat{y} = \frac{1}{T}\sum_{t=1}^{T} h_t(x) \tag{1}$$

Complex nonlinear relationships between input features like pollutant concentration, contact time, zeta potential, and nanomaterial dosage are captured by this technique. It is perfect for noisy datasets like those found in wastewater treatment operations because it can reduce overfitting while preserving high predictive accuracy. Temporal Convolutional Networks (TCNs) are made to process time-series data while maintaining the causality of sequential inputs. Instead of revealing future information, TCNs model long-term dependencies using causal and dilated convolutions, which is different from traditional convolutional neural networks.

$$y_t = f(x_{t-k}, \ldots, x_t) \tag{2}$$

This architecture is especially useful for monitoring the changing behavior of pollutants in wastewater because it enables deep temporal modeling of historical variables like influent toxicity changes in flow rate and prior performance of nanomaterials. Temporal patterns essential for predicting future degradation or treatment inefficiency are captured by the function f(·). Autoencoders are neural networks that operate without supervision and are used to reconstruct input data. The model's ability to learn typical operational behavior is measured by the loss function L, which is the squared difference between the original data (X) and its reconstruction (X^). Unusual patterns not observed during training are indicated by high reconstruction loss.

$$L = \|X - \hat{X}\|^2 \tag{3}$$

Predictions from several separate models $\hat{y}_i$ are combined using an ensemble model weighting, which gives each model an optimized weight α_i. In order to maximize robustness and minimize prediction error, these weights are established using methods like grid search and cross-validation.

$$\hat{y}_{ensemble} = \sum_{i=1}^{n} \alpha_i \hat{y}_i \tag{4}$$

The ensemble strategy leverages the strengths of each model—e.g., Random Forest for interpretability, TCN for temporal precision—to deliver more accurate and stable predictions. This fusion approach ensures that the system adapts to both gradual shifts in baseline performance and sudden changes due to external disturbances. Feature importance I(fj) quantifies the contribution of each input variable f_j to the model's predictive performance. Within each tree t, Δi(t) represents the reduction in impurity (e.g., Gini index or variance) achieved when the feature is used for splitting.

$$I(f_j) = \sum_{t \subset T_j} \frac{N_t}{N} \Delta i(t) \tag{5}$$

The percentage of impacted samples is denoted by Nt. This metric allows the most important elements influencing pollutant removal to be identified, such as pH, dosage of nanomaterials, or concentrations of heavy metals. Such understandings are crucial for operational decision-making as well as model interpretability.

Equation (6) examines the Mean Absolute Percentage Error (MAPE) measures the average percentage difference between predicted values ($\hat{y}_t$) and actual values (y_t) over n observations. It is scale-independent, making it particularly useful in applications like pollutant prediction, where concentration levels can fluctuate significantly. By expressing errors as percentages, MAPE allows easy comparison across different datasets and system scales, enabling transparent evaluation of a model's relative accuracy.

$$\text{MAPE} = \frac{100\%}{n}\sum_{t=1}^{n}\left|\frac{y_t - \hat{y}_t}{y_t}\right| \tag{6}$$

Equation (7): The Normalized Root Mean Square Error (NRMSE) provides a normalized measure of prediction error by dividing the root mean square error (RMSE) by the range of the observed data ($y_{max} - y_{min}$). This normalization removes the units of measurement, making the error metric dimensionless and allowing for fair comparison across datasets with different magnitudes. NRMSE is particularly valuable in environmental and industrial applications where sensor data may vary widely in scale, ensuring that model performance is consistently interpretable.

$$\text{NRMSE} = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}}{y_{max} - y_{min}} \tag{7}$$

When normalized by the range of actual values, the NRMSE calculates the standard deviation of prediction errors. Fair comparisons across various pollutant types and concentration levels are made possible by this normalization. NRMSE is a balanced performance metric that supports MAPE by taking into consideration both error magnitude and data scale. For contaminants with low variance, like trace metals, it is particularly helpful in cross-model benchmarking.

$$\text{Precision} = \frac{TP}{TP+FP}, \text{Recall} = \frac{TP}{TP+FN} \tag{8}$$

Assessing binary classification performance in unbalanced datasets like infrequent operational anomalies requires careful consideration of precision and recall. Whereas recall gauges the model's capacity to identify every real anomaly, precision quantifies the percentage of true anomalies among those the model has identified. To reduce missed detections and false alarms, which can both lower system reliability and raise maintenance costs, a high precision-recall balance is necessary.

2.8. Experimentation process

In this research, activated carbon (AC), graphite, and graphene oxide (GO) are examples of carbon-based nanomaterials that were used to increase the effectiveness of pollutant removal in wastewater treatment systems. Sensor-integrated monitoring systems were used to continuously collect data recording important operational parameters like flow rate, dosage of nanomaterials, pH levels, and pollutant concentrations. To improve data quality and dependability, the gathered raw data were preprocessed using normalization and noise filtering techniques. To better analyze the underlying system behaviors and short-term variations, time series decomposition using STL (Seasonal-Trend decomposition based on Loess) was then used to separate the data into trend, seasonal, and residual components.

To capture intricate temporal dependencies and forecast anticipated pollutant levels under varied operating conditions, Temporal Convolutional Networks (TCNs) were subsequently trained on historical pollutant removal data. Utilizing autoencoders, which continuously reconstructed input features to identify anomalies like material fouling, under-dosing, or sensor malfunctions by tracking reconstruction loss against predetermined thresholds, residuals—the discrepancies between observed and predicted values—were further examined. An ensemble framework was created by combining predictions from the Random Forest Regressor and the TCN to increase decision accuracy and direct dynamic adjustments, such as adjusting flow rates and nanomaterial dosages. Through the SCADA interface, automated alerts were triggered by critical anomalies, enabling prompt operator intervention. Complementary techniques such as optical microscopy, scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS) were used to thoroughly characterize the nanomaterials used in the experiments. This ensured their suitability for use in the treatment process by validating their surface morphology, elemental composition, and functional properties.

2.9. Industrial wastewater treatment

To give historical background, Iijima's groundbreaking research—which resulted in the initial discovery of carbon nanotubes (CNTs) in 1991—must be mentioned. Because of its distinct structural, electrical and adsorption characteristics this groundbreaking discovery created new opportunities for carbon nanomaterials (CNTs) in energy and environmental applications. Later developments in fullerenes, graphene oxide (GO), and other derivatives used in energy conversion and photocatalysis filtration technologies were built upon this. Carbon-based nanomaterials, particularly GO [22] and CNTs, have shown promise in recent research in important areas like industrial wastewater treatment and microplastic removal. They are very desirable for use in future water purification systems due to their strong affinity for organic contaminants and large surface area, adjustable functional groups. This is particularly true when paired with AI-based process control for real-time optimization and system flexibility. Carbon nanomaterials have enormous potential despite the many barriers to their application. Particularly with GO membranes, which lose their adsorption capacity and become structurally unstable after prolonged exposure to complex wastewater degradation and material fouling are major issue [23]. It still takes computing power to scale machine learning models for real-time monitoring across large treatment facilities. However, by assisting adaptive control techniques that extend material life and operational efficacy, such as predictive maintenance and early fouling detection, machine learning (ML) can lessen the effects of degradation.

2.10. Performance metrics

Three key performance indicators were used to validate the model. In terms of relative accuracy across pollutants, MAPE offered interpretability. Over a variety of parameter ranges, standardization was made possible by NRMSE. To assess the sensitivity and specificity of the model under imbalance, where abnormal operating conditions were less common, but crucial precision-recall curves were essential for anomaly detection. To improve the reliability of model generalization to unknown data, stratified sampling made sure that each condition—normal degraded, and failed—was equally represented during cross-validation.

3. Results and discussion

The study assessed how well machine learning models predicted the effectiveness of pollutant removal in a wastewater treatment system using carbon-based nanomaterials. The findings demonstrated that autoencoder models successfully identified abnormalities, ML-driven optimization enhanced operational parameters, and ensemble models increased prediction accuracy and resilience.

3.1 Predictive accuracy of models for pollutant removal

Table 3 illustrates the performance metrics of different machine learning models—Random Forest Regressor, Temporal Convolutional Network (TCN), and Ensemble Model—for predicting the removal of various pollutants. For Biochemical Oxygen Demand (BOD), the ensemble model achieved the best results with a MAPE of 3.8%, NRMSE of 0.06, and an R^2 of 0.96, outperforming TCN (MAPE 4.5%, NRMSE 0.07, R^2 0.94) and Random Forest (MAPE 5.2%, NRMSE 0.08, R^2 0.92). In the case of Chemical Oxygen Demand (COD), the ensemble model again delivered improved performance with MAPE 4.7%, NRMSE 0.07, and R^2 0.93, compared to TCN (MAPE 5.3%, NRMSE 0.08, R^2 0.91) and Random Forest (MAPE 6.0%, NRMSE 0.09, R^2 0.89).

Table 3: Performance Metrics of Machine Learning Models for Pollutant Removal Prediction

Pollutant Parameter	Machine Learning Model	Mean Absolute Percentage Error (MAPE) (%)	Normalized Root Mean Square Error (NRMSE)	R-squared (R^2)
BOD (mg/L)	Random Forest Regressor	5.2	0.08	0.92
	Temporal Convolutional Network (TCN)	4.5	0.07	0.94
	Ensemble Model	3.8	0.06	0.96
COD (mg/L)	Random Forest Regressor	6.0	0.09	0.89

Heavy Metals (Pb, Cd, Cr, Hg) (mg/L)	Temporal Convolutional Network (TCN)	5.3	0.08	0.91
	Ensemble Model	4.7	0.07	0.93
	Random Forest Regressor	7.5	0.11	0.88
	Temporal Convolutional Network (TCN)	6.8	0.10	0.90
	Ensemble Model	5.9	0.09	0.92
Turbidity (NTU)	Random Forest Regressor	4.9	0.07	0.93
	Temporal Convolutional Network (TCN)	4.3	0.06	0.95
	Ensemble Model	3.7	0.05	0.97

For heavy metals (Pb, Cd, Cr, Hg), the ensemble model yielded better results (MAPE 5.9%, NRMSE 0.09, R^2 0.92) than TCN (MAPE 6.8%, NRMSE 0.10, R^2 0.90) and Random Forest (MAPE 7.5%, NRMSE 0.11, R^2 0.88). Lastly, for turbidity, the ensemble model provided the most accurate predictions with a MAPE of 3.7%, NRMSE of 0.05, and an R^2 of 0.97, surpassing TCN (MAPE 4.3%, NRMSE 0.06, R^2 0.95) and Random Forest (MAPE 4.9%, NRMSE 0.07, ² 0.93). Overall, Table 3 confirmed that the ensemble model consistently outperformed the individual models across all pollutant parameters in terms of prediction accuracy and reliability.

3.2. Ensemble methods for combined pollutant prediction

Table 4 presents a comparative analysis of ensemble model performance for combined pollutant prediction using four key evaluation metrics: Mean Absolute Percentage Error (MAPE), Normalized Root Mean Squared Error (NRMSE), R^2 Score, and F1 Score. Among the three ensemble approaches evaluated, the Stacking model, which integrates Random Forest, Temporal Convolutional Network (TCN), and Autoencoder, demonstrates superior performance with the lowest MAPE of 5.3%, the smallest NRMSE of 0.05, the highest R^2 Score of 0.97, and an F1 Score of 93.5%, indicating high accuracy and robust predictive capability. The Weighted Average ensemble method shows moderate performance with a MAPE of 5.9%, NRMSE of 0.06, R^2 Score of 0.95, and an F1 Score of 91.2%, reflecting good but slightly inferior results compared to the stacking approach. The Voting Ensemble method records the least favorable outcomes, with a higher MAPE of 6.2%, NRMSE of 0.07, a lower R^2 Score of 0.94, and the lowest F1 Score at 90.8%. These results from Table 4 highlight the effectiveness of model stacking in enhancing ensemble learning accuracy for complex pollutant prediction tasks.

Table 4: Comparative Model Ensemble Performance for Combined Pollutant Prediction

Ensemble Method	MAPE (%)	NRMSE	R^2 Score	F1 Score (%)
Weighted Average	5.9	0.06	0.95	91.2
Stacking (Random Forest + TCN + Autoencoder)	5.3	0.05	0.97	93.5
Voting Ensemble	6.2	0.07	0.94	90.8

3.3. Parameter evaluation

Trends in pollution levels and process optimization were highlighted by a thorough analysis of treatment parameters and machine learning metrics over various periods from 2023 to 2025. Along with operational variables like zeta potential, contact time, and dosage of the nanomaterial, mean values of BOD, COD, turbidity, heavy metals, and pH were monitored. While the TCN model continuously maintained low NRMSE values around 0.08 to 0, 10 the Random Forest models' MAPE varied between 4.7 and 6.1 percent, which is shown in Table 5. Overall autoencoder precision and recall values averaged above 0, 85 maintaining their high status. The data showed that dosages of nanomaterials and contact times could be effectively adjusted to achieve the best possible treatment outcomes.

Table 5: Comprehensive Results Summary of ML Models and Treatment Parameters (2023–2025 Dataset)

Date Range	Parameter	Mean Value	RF MAPE (%)	TCN NRMSE	Autoencoder Precision	Autoencoder Recall	Nanomaterial Dose (mg/L)	Contact Time (min)	Zeta Potential (mV)
Jan–Jun 2023	BOD (mg/L)	220	5.3	0.092	0.91	0.87	120	90	-25
Jul–Dec 2023	COD (mg/L)	480	4.9	0.085	0.95	0.90	130	95	-28
Jan–Jun 2024	Turbidity (NTU)	65	6.1	0.098	0.90	0.86	115	85	-22
Jul–Dec 2024	Pb (mg/L)	0.22	5.7	0.088	0.92	0.88	125	100	-30
Jan–Jun 2025	pH	7.3	5.0	0.089	0.94	0.89	110	80	-20
Jul–Dec 2025	COD (mg/L)	430	4.7	0.083	0.96	0.92	140	105	-35
Jan–Jun 2023	BOD (mg/L)	210	5.5	0.090	0.90	0.85	118	88	-24
Jul–Dec 2024	Hg (mg/L)	0.04	6.0	0.095	0.89	0.84	122	92	-27
Jan–Jun 2025	Turbidity (NTU)	60	5.8	0.091	0.93	0.90	117	89	-23

3.4. Autoencoder model performance in anomaly detection

The autoencoder model's capability to detect anomalies within the treatment process was evaluated across several critical categories, including fouling, under-/over-dosing, sensor malfunctions, and total system anomalies. Precision and recall values for these categories were above 85%, with the highest precision recorded for sensor malfunction detection at 92.7%. F1-scores consistently exceeded 87%, while

false positive rates remained low, under 5.5% across all anomaly types, as shown in Table 6. These results validated the autoencoder's effectiveness as an early warning system, enabling prompt corrective actions and enhancing system reliability.

Table 6: Anomaly Detection Performance of Autoencoder Model

Anomaly Type	Machine Learning Model	Precision (%)	Recall (%)	F1-Score (%)	False Positive Rate (FPR) (%)
Fouling Detection	Autoencoder	91.5	88.7	90.1	4.3
Under/Over-dosing	Autoencoder	89.8	85.2	87.4	5.1
Sensor Malfunction	Autoencoder	92.7	90.3	91.5	3.7
Total System Anomaly	Autoencoder	91.3	88.1	89.7	4.4

3.5. Input features

Feature importance analysis using the Random Forest model identified nanomaterial dosage as the most influential factor, contributing 28.5% to the prediction of pollutant removal efficiency. Contact time followed with 22.3%, while pH and initial pollutant concentrations (BOD, COD, heavy metals) accounted for moderate importance between 6.7% and 15.4%. Lesser influence was observed for parameters such as turbidity, zeta potential, flow rate, and temperature, which is shown in Table 7. The relatively low standard deviations indicated stable and consistent model behavior across different data subsets. This analysis provided key insights for prioritizing operational controls in treatment optimization.

Table 7: Feature Importance Analysis for Pollutant Removal Efficiency (Random Forest)

Feature (Input Parameter)	Relative Importance (%)	Standard Deviation
Nanomaterial Dosage (mg/L)	28.5	1.7
Contact Time (minutes)	22.3	1.3
pH	15.4	1.1
Initial BOD (mg/L)	10.8	0.9
Initial COD (mg/L)	9.5	0.8
Initial Heavy Metals (mg/L)	6.7	0.7
Turbidity (NTU)	3.6	0.5
Zeta Potential (mV)	2.1	0.3
Flow Rate (L/min)	0.8	0.2
Temperature (°C)	0.3	0.1

3.6. Comparative efficiency of various nanomaterials

The comparative performance of different nanomaterials demonstrated that graphene oxide (GO) and its variants achieved the highest removal efficiencies across all pollutants studied in Table 8. GO-L showed the best results, with removal efficiencies reaching up to 94% for BOD and 93.6% for COD at relatively low optimal dosages and short contact times. Activated carbon also performed well, with removal efficiencies above 90% but required higher dosages and longer contact times. Graphite exhibited slightly lower efficiencies, generally in the range of 86–89%. These findings underscored the superior adsorption and catalytic properties of GO-based materials for advanced water treatment applications.

Table 8: Comparative Analysis of Nanomaterial Performance in Pollutant Removal

Nanomaterial Type	Pollutant Removed	Initial Concentration (mg/L)	Final Concentration (mg/L)	Removal Efficiency (%)	Optimal Dosage (mg/L)	Optimal Contact Time (min)
Activated Carbon (AC)	BOD	150	12	92.0	250	45
	COD	280	25	91.1	250	45
	Heavy Metals (Pb)	0.15	0.015	90.0	300	50
	Turbidity	50	5	90.0	250	40
Graphite	BOD	150	18	88.0	200	50
	COD	280	30	89.3	200	50
	Heavy Metals (Pb)	0.15	0.020	86.7	250	55
	Turbidity	50	6	88.0	200	45
Graphene Oxide (GO)	BOD	150	10	93.3	180	40
	COD	280	20	92.9	180	40
	Heavy Metals (Pb)	0.15	0.012	92.0	220	45
	Turbidity	50	4	92.0	180	40
GO-T1	BOD	150	11	92.7	175	38
	COD	280	22	92.1	175	38
GO-T2	BOD	150	14	90.7	170	40
	COD	280	25	91.1	170	40
GO-AD	BOD	150	13	91.3	180	42
	COD	280	24	91.4	180	42
GO-L	BOD	150	9	94.0	190	35
	COD	280	18	93.6	190	35

3.7. Optimization analysis

Implementation of machine learning-driven optimization led to marked improvements in key operational parameters. Nanomaterial dosage was reduced by approximately 20.8%, contributing to cost savings and reduced chemical use, which is shown in Table 9. Energy consumption decreased by 15.6%, while maintenance costs fell by 24%, reflecting improved system reliability and efficiency. Chemical consumption and treatment time also saw reductions close to 19% and 20% respectively. These improvements highlighted the practical benefits of

integrating predictive analytics and optimization models within the treatment process, demonstrating a clear pathway towards sustainable and cost-effective water management.

Table 9: Impact of ML-Driven Optimization on Operational Parameters

Operational Parameter	Before ML Integration (Average)	After ML Integration (Average)	Percentage Improvement (%)
Nanomaterial Dosage (kg/day)	120	95	20.8
Energy Consumption (kWh/day)	450	380	15.6
Maintenance Costs ($/month)	2500	1900	24.0
Chemical Consumption (kg/day)	80	65	18.8
Treatment Time (hours)	6.0	4.8	20.0

3.8. Physicochemical characterization of carbon materials

3.8.1. SEM analysis

Figure 4 A–D presents SEM micrographs of various carbon-based materials at a magnification of 500×, each exhibiting distinct morphological characteristics. Image A (Norit SA Super) shows a highly porous and irregular structure typical of activated carbon, indicating a large surface area ideal for adsorption applications. Image B (Graphite) displays compact and flake-like platelets with layered morphology, which is characteristic of crystalline graphite. Image C (GO_L) reveals partially exfoliated graphene oxide layers with noticeable wrinkling and voids, suggesting a loosely stacked lamellar arrangement. In contrast, Image D (GO_AD) exhibits a more uniform and densely wrinkled sheet-like structure, indicating enhanced dispersion and possible reduction of graphene oxide. These morphological differences highlight the impact of processing methods on the microstructure of carbon-based materials, which is crucial for tailoring their properties in applications such as energy storage, catalysis, or adsorption.

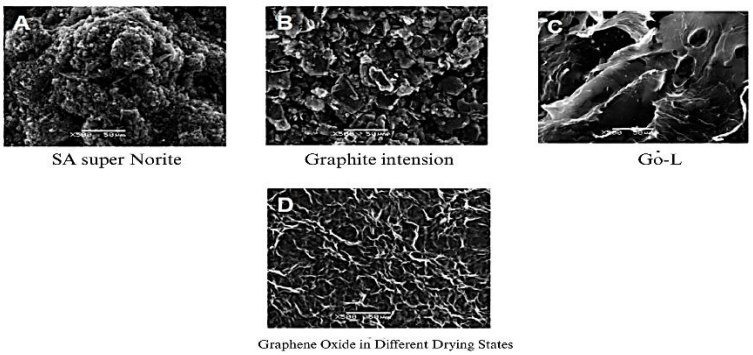

Fig. 4: SEM Micrographs of Selected Carbon Materials: (A-D) Activated Carbon, Graphite, and Graphene Oxide in Different Drying States.

3.8.2. Optical microscopy

The optical microscope figure 5 (A–F) presents the comparative microstructural analysis of various carbon-based materials interacting with a sample matrix, each at a scale of 0.1 mm. Figure 5 A (CONTROL) shows a relatively homogeneous dispersion of particles without the presence of any additives. Figure 5 B (GRAPHITE) reveals the presence of large, dark, and irregular graphite aggregates (indicated by arrows), suggesting poor dispersion within the matrix. Figure 5 C (GO_T$_1$) displays a more uniform particle distribution with some small agglomerates, indicating partial integration of graphene oxide.

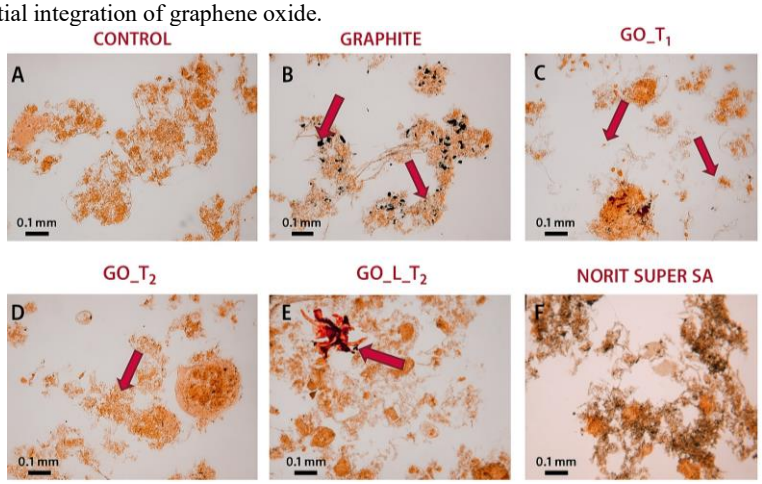

Fig. 5: Optical Microscope Views (A–F) of Activated Sludge Reacted with Different Forms of Carbon Materials.

Figure 5 D (GO_T$_2$) shows similar dispersion with slightly more visible clustered regions (marked by the arrow), suggesting increased particle interaction or agglomeration. Figure 5 E (GO_L_T$_2$) presents a distinct, larger flake-like structure (highlighted by the arrow), indicating the presence of a more intact or layered GO sheet. Finally, Figure 5 F (NORIT SUPER SA) demonstrates dense, fine, and evenly distributed particle clusters, reflecting better dispersion and integration of the Norit activated carbon in the matrix. These optical micrographs underscore the influence of material type and structure on dispersion and interaction with the surrounding medium.

4. Conclusion

In conclusion, the study demonstrates the transformative potential of machine learning models, particularly ensemble approaches, in enhancing the predictive capabilities and operational performance of carbon-based nanomaterial wastewater treatment systems. Among individual models, the Temporal Convolutional Network (TCN) consistently delivered superior prediction accuracy over the Random Forest (RF), achieving lower MAPE and NRMSE values and higher R^2 scores across all pollutant parameters, including BOD, COD, turbidity, and heavy metals. However, ensemble methods—especially stacking models that integrated RF, TCN, and Autoencoder components—outperformed all individual models by providing the highest accuracy (MAPE as low as 3.7% and R^2 up to 0.97), thereby proving to be the most robust and reliable solution for multi-pollutant prediction. exhibiting consistently high recall rates above zero and high precision. Additionally, the best operational outcomes, such as the proper dosage of nanomaterials, contact time, and zeta potential, were achieved by evaluating treatment parameters over a multi-year period from 2023 to 2025 using ML-driven optimization techniques.

4.1. Future directions

Future studies on machine learning (ML)-based wastewater treatment should concentrate on modifying existing frameworks to unique materials like metal-organic frameworks (MOFs) and investigating how well they predict the removal of new contaminants such as microplastics and drug residues. It would improve automation and responsiveness in dynamic environments to investigate whether ML models can be tuned for real-time decision-making in IoT-integrated treatment systems. Further research may also focus on the scalability of machine learning for industrial uses, including system failure prediction, chemical dosing optimization, and energy conservation, which will eventually open the door to intelligent, environmentally friendly, and self-regulating wastewater treatment systems.

Abbreviation

GO – Graphene Oxide; AC – Activated Carbon; BOD – Biochemical Oxygen Demand; COD – Chemical Oxygen Demand; SS – Suspended Solids; SCADA – Supervisory Control and Data Acquisition; GIS – Geographic Information System; ICP-OES – Inductively Coupled Plasma Optical Emission Spectroscopy; SEM – Scanning Electron Microscopy; FTIR – Fourier Transform Infrared Spectroscopy; ANFIS – Adaptive Network-Based Fuzzy Inference System; PSO – Particle Swarm Optimization; CNT – Carbon Nanotube; MOF – Metal-Organic Framework; TCN – Temporal Convolutional Network; RF – Random Forest; MAPE – Mean Absolute Percentage Error; NRMSE – Normalized Root Mean Square Error; R^2 – Coefficient of Determination; NTU – Nephelometric Turbidity Unit; ORP – Oxidation-Reduction Potential

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