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Artificial Neural Network (ANN)-Based Classification of Photocatalytic Dye Degradation Utilizing MATLAB

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ABSTRACT

This study applied MATLAB-based artificial neural network (ANN) methods to predict photocatalytic dye degradation. Standard experimental techniques need help to capture process complexity, hindering accurate predictions. Leveraging machine learning, specifically ANN, and optimal design and input variables, this research overcame challenges to create a prediction model. Real-life data were used to evaluate the model's accuracy, offering valuable insights into effective and affordable wastewater treatment approaches. The Levenberg-Marquardt (LM) algorithm was employed in this study's ANN architecture and was well-suited to non-linear regression problems. Experimental data on photocatalytic dye degradation were used as real-life data that serve as the basis for evaluating the accuracy and performance of the prediction model. The results showed that the ANN models performed well, with R^2 values ranging from 0.9917 to 0.99814 in training,validation, and testing for the selected structure (3-10-1) predictions for photocatalytic dye degradation. This study successfully developed a highly accurate ANN model for predicting photocatalytic dye degradation during wastewater treatment, demonstrating machine learning's promising potential for optimizing such environmental processes.

INTRODUCTION

Synthetic dyes in various industries, such as textile fibers, cosmetics, paper, tanneries, food, leather, and pharmaceuticals, have led to a daunting problem in water treatment processes [1,2]. These dyes are known for their high aromaticity, low biodegradability, toxicity, chemical stability, and even

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carcinogenicity, making them major water pollutants [3]. Moreover, they also hinder light penetration and reduce photosynthetic activity, which leads to a deficiency in the dissolved oxygen content of the water [4]. In response to these concerns, various approaches, such as adsorption, nanofiltration, ozonation, coagulation, biodegradation, and phytoremediation, have been implemented to remediate these pollutants [5].

These conventional techniques, however, frequently have downsides, including high costs, destructiveness, difficulty in handling, and the production of sludge as a byproduct. Even though these techniques have been used to clean water, there is a rising need for more effective and environmentally friendly alternatives. Analyzing and comprehending complex data related to dye degradation processes is essential for successfully addressing this challenge. Due to the intricate nature of the underlying chemical interactions, interpreting dye degradation data can be challenging and complicated. Conducting lab tests and studies on photodegradation activity may take time and effort. As a result, there is a need for approaches and tools that can accelerate data processing and make predictions based on experimental findings. Artificial neural networks (ANN) are a promising prediction approach [6]. The non-linear correlations and complexity in the dye degradation process can be captured using ANN models.

Machine learning is a powerful tool that ANN may use to efficiently analyze experimental data, identify significant patterns, and generate precise predictions. Under various operating conditions, the primary objective of dye degradation is to attain a high removal percentage. The dynamic interaction between input and output parameters in the degradation mechanism makes it difficult to predict the target using mathematical models. Computational data models are more versatile for simulating large datasets than mathematical ones [7]. In modeling the system, artificial intelligence prediction methods such as random forest [8,9], adaptive neuro-fuzzy inference system [10–12], least square support vector regression [13-15], and ANN [6,16–18] have recently been effectively employed. The ANN model may be applied to any complicated engineering system based on cognitive nervous processing because of its resilience, durability, and nonlinearity. Furthermore, without prior conventions, the ANN model can learn from any experimental dataset to overcome complex, non-linear, and multi-dimensional functional relationships [7]. ANNs are the preferred prediction model in learning algorithms because they can comprehend the complex non-linear relationship between process parameters and their outputs [19].

Oladipo et al. [20] used ANN to model the degradation of organophosphorus pesticides in a single and binary system. Additionally, Amani-Ghadim & Dorraji [21] also used ANN to model the photodegradation of dye over ZnO photocatalysts, with a 3-layer perceptron neural network effectively modeled the photodegradation of dye with accurate prediction values. Das et al. [22] also employed ANN to predict carbamazepine photodegradation over TiO-ZnO photocatalysts. The primary objective of this research is to apply an ANN model using MATLAB, which can predict the photocatalytic degradation of dyes with high precision. Additionally, this study aimed to evaluate the performance and accuracy of the ANN model by comparing it to actual data. To achieve these objectives, the research sought a reliable and cost-effective approach to remediating synthetic dyes from industrial effluents and reducing the environmental impact of industrial waste discharge.

EXPERIMENTAL

The study was divided into three stages. The first was data collection and preprocessing, which involved tabulating and organizing two data types in a spreadsheet: input and output. The second part dealt with ANN model selection and architecture. The hidden layer was specified, and the data was divided into three subsets: training, validation, and testing. Lastly, the final section covered ANN model training and validation. In this section, the network with the Levenberg-Marquardt algorithm was trained and verified to be optimal. Specifically, the dataset consists of 36 samples, and we used a 3-10-1 architecture. The epochs were determined through trials to balance learning accuracy and computational efficiency. Fig.1 depicts a flowchart for the overall methodology in this study.

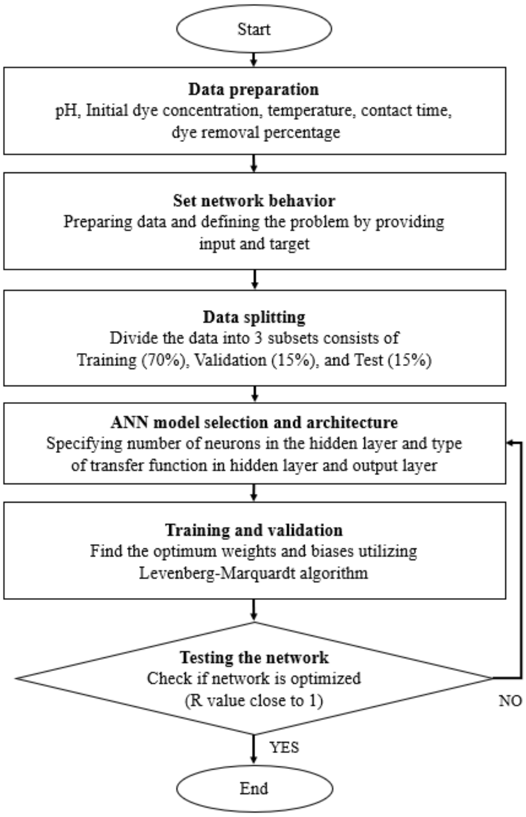

Fig.1. Flow chart of overall methodology

Data collection and preprocessing

The data was tabulated and organized inside a spreadsheet file. It consists of data input variables (dye initial concentration, contact time, photocatalyst composition) and single output (dye removal percentage). The spreadsheet file data for input and output was selected and set into matrix rows.

ANN model selection and architecture

The data was divided into three subsets: training, validation, and testing, which MATLAB randomly assigned: 70% training, 15% validation, and 15% testing. The hidden layer was thenspecified after the data had been divided into three subsets. This neuron network can be adjusted over time to achieve optimal architecture. In an ANN, the hidden layer is a processing layer between the input and output layers. Data from the input was received, and mathematical procedures were used to modify and extract relevant details. The complexity and highperformance of neural networks may be linked to their hidden layers. The ANN's output layer generates the network's final prediction or output based on the data processed by the hidden layer[23–25]. The gathered data was then used to calculate an appropriate value or response to the task.

ANN model training and validation

The data was then trained using the Levenberg-Marquardt algorithm (trainlm). According to [26], the "trainlm" method uses Levenberg-Marquardt optimization to revise the network's weights and biases. The "trainlm" algorithm tends to converge quickly. The validation process ended when the network's generalization level stopped increasing during training. There was no impact on network training from the testing vector, but it did assist in confirming the validity of the network's generalization. Following ANN training, the performance, training state, error histogram, regression, and fit plots were obtained for further analysis and discussion. Different hidden value sets with regression values were compared for optimization, and the network architecture was selected and finalized. Based on this result, we can determine which ANN architecture is most effective (coefficient of determination (R^2) value close to 1).

RESULTS AND DISCUSSION

The findings of this research were organized into four categories: descriptive analysis, artificial neural network (ANN) design, ANN model development, and model performance evaluation. Photocatalytic dye degradation parameters were used as prediction inputs, including initial dye concentration, contact time, and photocatalyst composition. The study used three photocatalyst compositions: chitosan, titanium dioxide, and zirconium dioxide. The composition was labeled with set numbers: 1 (chitosan), 2 (chitosan and titanium dioxide), and 3 (chitosan, titanium dioxide, and zirconium dioxide).

Descriptive analysis

The descriptive analysis is tabulated in Table 1. It outlines the fundamental characteristics of the data in this study. It also provides basic overviews of the sample and measurements, including the minimum (min) values, maximum (max) values, mean values, and standard deviation values of the initial concentration (mg/l), time (min), and set of photocatalyst composition.

Table 1. Descriptive analysis for operating conditions of photocatalytic dye degradation

Inputs	Min	Max	Mean	SD
Initial concentration (mg/l)	10	30	19.44	8.41
Contact time (min)	30	120	75.00	34.65
Set of photocatalyst composition	1	3	2.00	0.82

These statistical measures are crucial when preparing and preprocessing data for ANN training. Normalizing, centering, and standardizing input data helps to ensure a more stable and effective training process, improving the network's ability to generalize to new, previously unseen data. It is a common practice in machine learning to preprocess data in a way that facilitates the learning process for neural networks and other models. The operating conditions shown in Table 1 were considered to achieve the desired percentage removal values.

The model used in this study has one input layer, one hidden layer with nodes, and one output layer. The maximum value of the correlation coefficient was used to calculate the number of nodes in the hidden layer [27]. As a result, several network architectures were examined to identify the optimal number of hidden layers and nodes in each. Fig.2 illustrates the current study's neural network structure for the photocatalytic degradation model. The training process was configured using input and output data. As a result, the data was divided into three categories: training (70%), validation (15%), and testing (15%).

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This training data was used to learn and adjust network weights by minimizing an error function. Thirty-six samples were used for ANN modeling, and the datasets were randomly divided for training, validation, and testing in MATLAB. It included five samples for validation, five for testing, and 26 for training. The coefficient of determination (R^2) was obtained through regression analysis. It refers to the ratio of the variation in the dependent variable (output) that can be predicted based on the independent variables (input) [28]. The R^2 value indicated which network would be selected as the optimal structure, with an R^2 value close to 1.

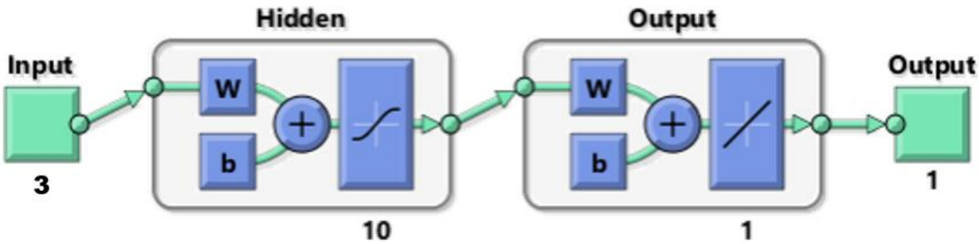

Fig.2. ANN architecture for photocatalytic dye degradation.

ANN model

The ANN models were built to compare the measured and predicted values by ANN using the optimal ANN architecture shown in Fig.2. The characteristic data (input) of initial dye concentration, contact time, and photocatalyst composition were combined into one data set. Since we have 36 samples used, 36 data sets were presented. Thus, the plot of percentage removal (%) versus the number of data sets was generated to visualize the relationship between measured and predicted values.

According to the plot in Fig.3, the developed ANN models exhibited comparable deviations from the measured values with an average percentage error of 0.30%. In general, the ANN accurately represented the actual measured value. This is true, even though the developed models showed constant variations across different data sets. Hence, the developed models showed the neural network models' proficiency in accurately predicting photocatalytic dye degradation percentage removal.

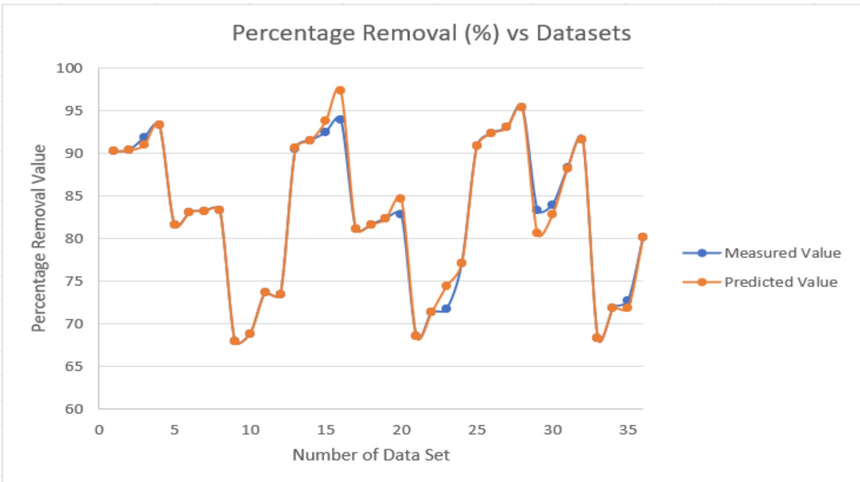

Fig.3. Percentage removal (%) versus number of data sets for selected ANN architecture (3-10-1).

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Model performance evaluation

The confusion matrix, as shown in Fig.4, details the performance of our ANN model in predicting the level of photocatalytic dye degradation. The matrix is structured as follows:

- True Positives (TP = 25): The model correctly predicted those 25 instances with high degradation, which was more than 80%.
- True Negatives (TN = 11): In the model, 11 instances were correctly predicted with low degradation (less than or equal to 80%).
- False Positives (FP = 0): There were no false positives from the model. It did not predict low degradation as high.
- False Negatives (FN = 0): No instance was incorrectly predicted, with instances having high degradation as low.

All predictions are True Positives (TP). Therefore, a high degree of accuracy implies that the model is very effective in recognizing low and high levels of degradation without any error, thus endowing it with a reliable tool for monitoring and controlling the dye degradation process in industrial practices. After determining the optimal number of neurons for the hidden layer via trial and error, the network underwent training for ten iterations. The linear plots of the ANN validations versus the output are shown in Fig.5. Each model shown has a different hidden layer. Based on this condition, the optimal structure or ANN architecture for the photocatalytic dye degradation was determined to be 3-10-1 with an R^2 value of 0.99088. The R^2 values for training, testing, and validation were 0.99814, 0.99223, and 0.9917, respectively. Hence, the anticipated output of the ANN demonstrated a strong correlation between the percentage of dye degradation achieved and the actual experimental results.

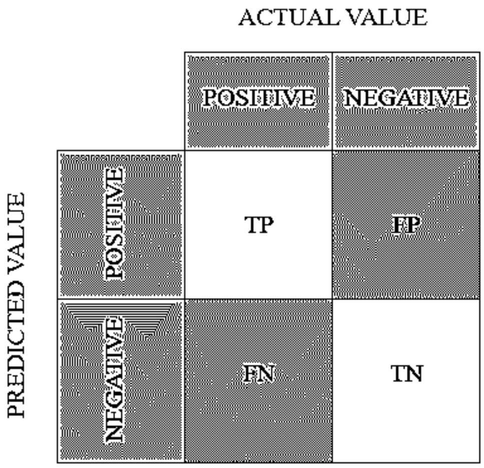

Fig.4. Confusion matrix

Fig.6 shows the error histogram with 20 bins predicted by the neural network. ANN forecasted the outcome and verified the measured data. The R^2 must reach 1, and there will always be an error between the predicted and experimental results [29]. The slightest error histogram can be seen in Fig.6(b), with nine total zero errors and fewer error spikes compared to other ANN architecture. This finding supported the model, which is 3-10-1, as the selected ANN model compared to another model. The histogram provides a quick overview of how errors are distributed across the dataset. If the histogram is symmetrically distributed around zero, it suggests that the ANN tends to be unbiased in its predictions. By examining the distribution of errors, the overall performance of the ANN could be assessed. Ideally, a histogram centered around zero indicates that the predicted values are close to the actual values.

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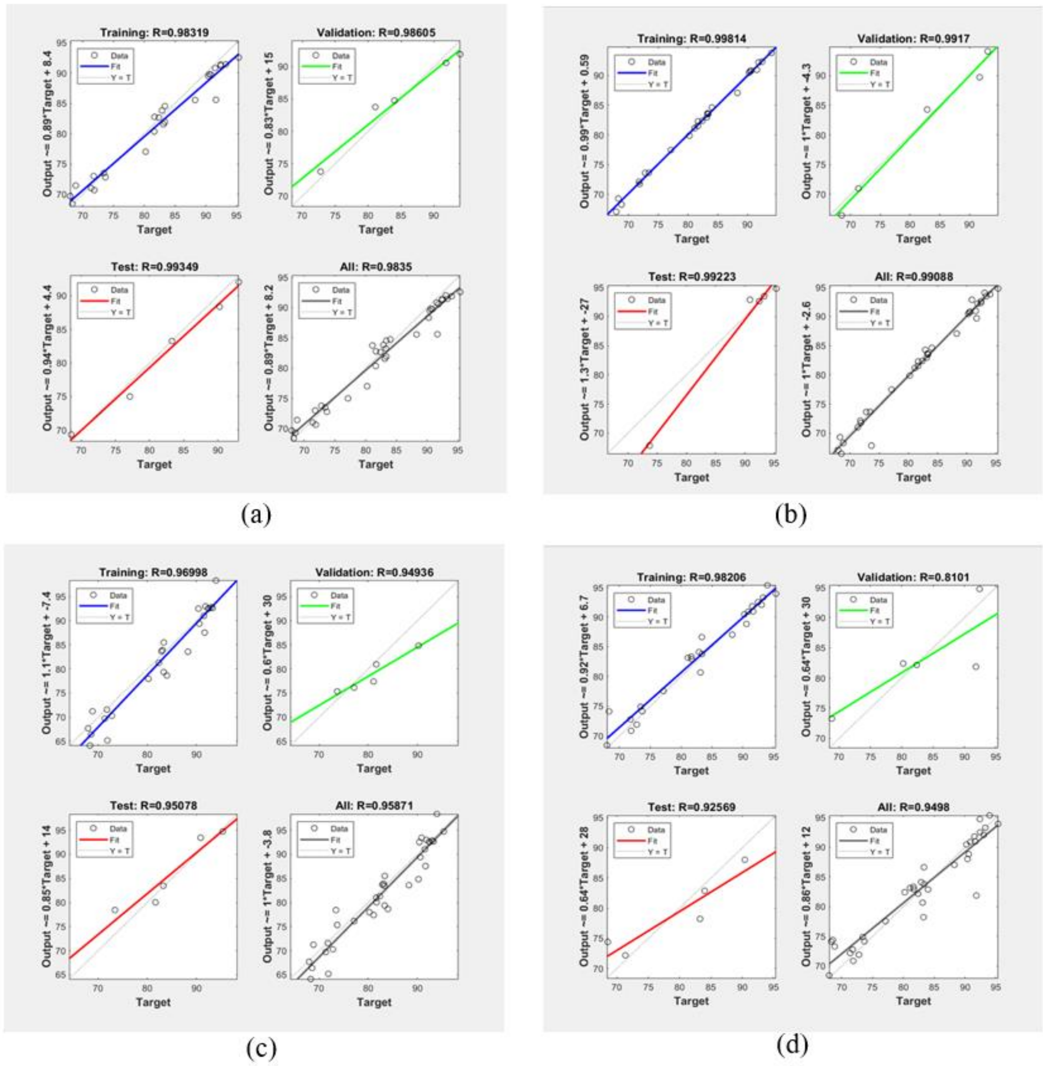

Fig.5. Regression analysis at various ANN architecture, (a) 3-5-1, (b) 3-10-1, (c) 3-15-1, and (d) 3-20-1.

Furthermore, mean squared error (MSE) measures how close the predicted values are to the actual values. It enables us to determine how well the network generates accurate predictions. A lower MSE indicates that the predictions are more relative to the actual data, indicating better performance. Fig.7 shows the MSE for training, validation, and testing. Fig.7(b) shows that the training was stopped with a mean square error of 2.2654, the lowest value compared to the MSE presented by the other architectures. This finding suggested that the ANN's projected outputs are close to experimental results (measured values).

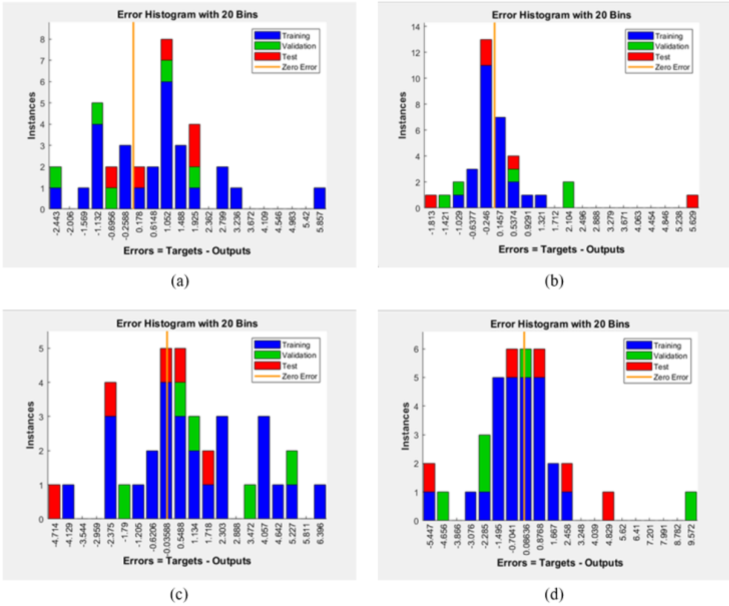

Fig.6. Error histogram for percentage removal predicted by (a) 3-5-1, (b) 3-10-1, (c) 3-15-1, and (d) 3-20-1 ANN architectures.

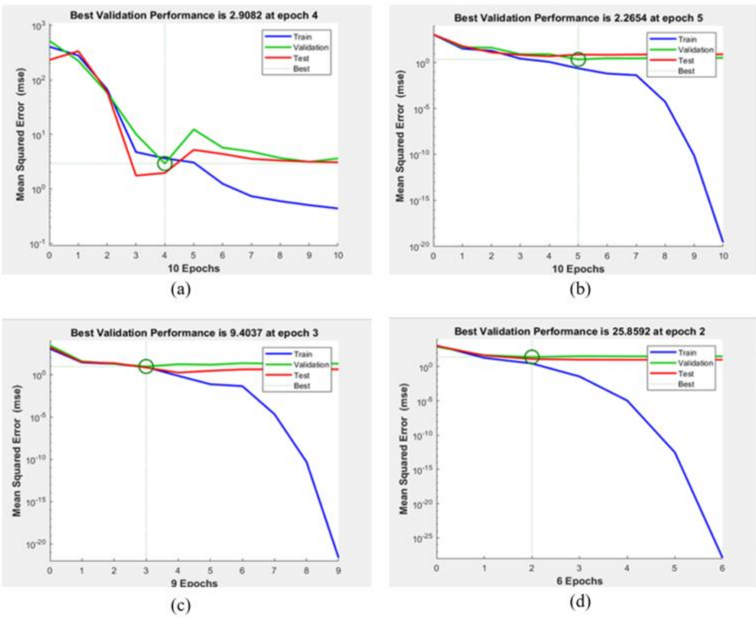

Fig.7. Mean Square Error (MSE) for (a) 3-5-1, (b) 3-10-1, (c) 3-15-1, and (d) 3-20-1 ANN architectures.

The R^2 and MSE performances of other ANN architectures are presented in Table 2. Of important significance, the 3-10-1 architecture gave better results of maximum R^2 values in all phases: training, testing, and validation, with a low MSE of 2.2654. The architecture has high accuracy and reliability in modeling photocatalytic dye degradation. This architecture remains effectively balanced in complexity and learning capacity, making it best suited in predictive environmental modeling where precision is of high value to operations and decision-making activities.

Table 2. ANN architecture performance summary

ANN Architectures	R^2 (Training)	R^2 (Test)	R^2 (Validation)	R^2 (All)	MSE
3-5-1	0.98319	0.99349	0.98605	0.98350	2.9082
3-10-1	0.99814	0.99223	0.99170	0.99088	2.2654
3-15-1	0.96998	0.95078	0.94936	0.95871	9.4037
3-20-1	0.98206	0.92599	0.81010	0.94980	25.8592

CONCLUSION

This study applied MATLAB-based artificial neural network (ANN) methods to predict photocatalytic dye degradation in developing a precise and cost-effective wastewater treatment prediction model. Photocatalytic dye degradation parameters include initial concentration, time, and photocatalyst composition. The coefficient of determination (R^2), error histogram for % removal, and mean square error (MSE) were used to evaluate the performance of the models. The results revealed that the ANN models have a high prediction accuracy; the selected ANN architecture (3-10-1) showed $R^2 = 0.99088$, nine total of zero errors, and had fewer spikes of error compared to other ANN architectures as well as the lowest MSE value of 2.2654, indicating a similarity between measured and predicted values for the photocatalytic dye degradation removal percentage. This study successfully developed a highly accurate ANN architecture for predicting photocatalytic dye degradation during wastewater treatment, demonstrating machine learning's promising potential for optimizing such environmental processes.

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CONFLICT OF INTEREST STATEMENT

The authors agree that this research was conducted without any self-benefit, commercial, or financial conflicts and declare the absence of conflicting interests with the funders.

AUTHORS' CONTRIBUTIONS

Each contribution can be recognized as follows: Mohd Arif Effandi Samawi conducted the research work and article writing. Mohd Fadhil Majnis and Mohd Azam Mohd Adnan conceptualized the central research idea and provided the theoretical framework. Mohd Fadhil Majnis and Mohd Azam Mohd Adnan anchored the review and finalized the article submission.

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