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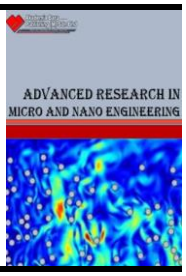

Artificial Neural Network-driven Optimization of Fe_3O_4 Nanoparticles/PVDF Macrospheres in Fenton-like System for Methylene Blue Degradation

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ABSTRACT

Efficient degradation of industrial dyes remains a critical challenge in environmental engineering. This study introduces a novel Fe_3O_4 nanoparticles/PVDF macrospheres in a Fenton-like system, optimized using an Artificial Neural Network (ANN) for the degradation of Methylene Blue (MB). A feedforward backpropagation neural network model to optimize and predict the performance of this advanced oxidation process under various operational conditions. The model was trained, validated, and tested with robust datasets, demonstrating high predictive accuracy and generalization capability. The Mean Square Error (MSE) and Root Mean Square Error (RMSE) during testing were 0.0200 and 0.1414, respectively, indicating precise predictions. The coefficient of determination (R^2) and correlation coefficient (R) were exceptionally high at 0.9744 and 0.9871, affirming the model's ability to capture the underlying dynamics of the degradation process effectively. The ANN-driven approach not only enhanced the efficiency of the MB degradation process but also provided significant insights into the scalability and applicability of the Fe_3O_4/PVDF system for practical water treatment solutions. This study underscores the potential of integrating advanced machine learning techniques with chemical engineering processes to achieve sustainable and efficient environmental management solutions, particularly for the treatment of recalcitrant wastewater contaminants.

1. Introduction

Water pollution represents a significant environmental issue, with dyes from the textile, paper, and other industries posing a major threat to aquatic ecosystems and human health [1,2]. Methylene Blue (MB), a widely used cationic dye, is known for its persistence and toxicity [3]. Addressing this

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challenge is crucial for achieving the United Nations' Sustainable Development Goals (SDGs), particularly SDG 6 (Clean Water and Sanitation) [4]. Conventional dye removal methods such as adsorption, coagulation/flocculation, and biological treatment often suffer from drawbacks that limit their widespread implementation [5]. Adsorption may be hindered by the availability [6–9] and cost of effective adsorbents as well as the challenges associated with regeneration and disposal. Coagulation and flocculation can generate hazardous sludge, which requires additional treatment and disposal [10,11]. Biological methods may be less effective against the intricate and diverse dye structures commonly found in textile and paper industry effluents, and their performance may be sensitive to fluctuations in process conditions [12,13].

Advanced Oxidation Processes (AOPs), particularly Fenton-like reactions, are promising solutions for dye degradation because of their powerful oxidative potential [14]. These processes rely on the generation of highly reactive hydroxyl radicals (•OH), which can non-selectively degrade a wide variety of organic pollutants including recalcitrant dyes [15]. The classical Fenton reaction involves the reaction between ferrous ions (Fe^{2+}) and hydrogen peroxide (H_2O_2) to produce hydroxyl radicals [16]. However, homogeneous Fenton processes have limitations, such as a narrow working pH range, the need for post-treatment sludge removal, and difficulties in catalyst recovery [16]. Heterogeneous Fenton-like catalysts have attracted considerable attention to overcome these drawbacks. These catalysts utilize solid-phase materials, which often contain iron-based species, to activate H_2O_2 and generate Reactive Oxygen Species (ROS) [17]. Among various heterogeneous systems, Fe_3O_4 nanoparticles supported on PVDF macrospheres offer distinct advantages [18]. Fe_3O_4 nanoparticles possess intrinsic catalytic activity, high surface area, and the ability to undergo redox cycling between the Fe^{2+} and Fe^{3+} states, which is crucial for the Fenton-like reaction. PVDF macrospheres provide a robust, chemically inert, and porous support, which significantly enhances the performance of Fe_3O_4 catalysts [19]. The immobilization of Fe_3O_4 nanoparticles on PVDF minimizes nanoparticle agglomeration [20]. Agglomeration can lead to reduced surface area and catalytic activity [21]. PVDF's structural properties of PVDF promote excellent Fe_3O_4 dispersion, ensuring that the catalyst maintains its high surface area and reactivity [22]. Furthermore, the macroporous structure of PVDF facilitates the diffusion of reactants and products within the catalyst system, further enhancing the reaction efficiency [22].

The precise functioning of Fenton-like reactions in conjunction with Fe_3O_4/PVDF can be intricate and influenced by factors such as the pH and reactant concentrations [19]. A basic representation comprises the following stages: surface reactions, in which Fe^{2+} species situated on the Fe_3O_4 surface react with H_2O_2, leading to the formation of Fe^{3+} and hydroxyl radicals (•OH), which involve the reduction of Fe^{3+} back to Fe^{2+} through various pathways, including reactions with more H_2O_2 or organic intermediates, guaranteeing the continuation of the catalytic cycle; and finally, dye degradation, which occurs when the highly reactive •OH radicals attack dye molecules, resulting in their breakdown into smaller, less harmful compounds [23,24]. This Fe_3O_4/PVDF system offers several key advantages over the conventional Fenton processes. Heterogeneous Fenton-like catalysts typically operate over a broader pH range, reducing the need for extensive pH adjustment. Minimal Fe leaching minimizes the need for post-treatment sludge handling and decreases secondary waste generation [25,26]. The magnetic properties of Fe_3O_4, paired with the macrosphere support, facilitate simple catalyst separation, reuse, and enhance process economics. Additionally, the PVDF support safeguards Fe_3O_4 nanoparticles from deactivation mechanisms, such as aggregation, improving catalyst lifespan, and maintaining long-term efficiency.

The efficiency of Fenton-like reactions, which is influenced by several operational parameters, is a significant challenge for optimization. Variables such as initial pH, catalyst loading, and H_2O_2 dosage display complex, non-linear interactions that directly affect dye degradation performance.

Conventional optimization methods can be time-consuming and resource-intensive, making them inadequate for capturing the intricate relationships between variables [27]. Artificial Neural Networks (ANNs) offer a powerful alternative that enables data-driven modelling and optimization of complex processes. ANNs are computational models inspired by biological neural networks, and their ability to learn from experimental data makes them suitable for analyzing systems, such as Fenton-like reactions, where the interplay of multiple factors is difficult to model using conventional mathematical approaches. In this study, a feedforward backpropagation ANN was employed, which consisted of an input layer, one or more hidden layers, and an output layer. The input data represent factors such as the initial pH, catalyst loading, and H_2O_2 dosage, and the output layer provides the predicted dye decolorization efficiency. The back-propagation algorithm is a critical component for training Artificial Neural Networks (ANNs). This process begins by inputting data into the network, which then performs calculations through the hidden layers to generate a predicted output. The predicted output was then compared with the actual experimental outcome, and the error value was determined. The error is then propagated backward through the network, and the weights and biases associated with each neuron connection are adjusted to reduce the error in the subsequent iteration. This process was repeated with new input data until the error was minimized, and the ANN could accurately predict the dye degradation results. Once trained, a well-designed ANN can accurately forecast the dye degradation outcomes for various combinations of input parameters. This predictive ability facilitates efficient optimization. Instead of relying on extensive trial-and-error experiments, an ANN model can quickly explore multiple scenarios [28]. This enables the identification of the optimal conditions that maximize dye degradation efficiency while minimizing resource consumption. The use of an ANN streamlined the optimization process, potentially leading to significant enhancements in the performance and sustainability of the Fe_3O_4/PVDF Fenton-like process. Although Artificial Neural Networks (ANNs) have been utilized in diverse optimization scenarios for wastewater treatment, their application in optimizing Fe_3O_4/PVDF Fenton-like systems for the degradation of methylene blue is relatively scarce. Existing research has generally concentrated on different pollutants or alternative catalyst systems. To bridge this knowledge gap, the current study aimed to develop an ANN-based model capable of predicting and optimizing the decolorization efficiency of methylene blue using a Fe_3O_4/PVDF Fenton-like process. This model incorporates experimental data pertaining to key factors, such as the initial pH, catalyst loading, and H_2O_2 dosage, with dye decolorization serving as the primary response variable. By harnessing the predictive power of the ANN, this research endeavours to identify the optimal process conditions that maximize decolorization efficiency. This research contributes to the advancement of sustainable and efficient dye removal technologies, specifically addressing the persistent challenges of methylene blue contamination.

2. Material and Methods

2.1 Material

The chemicals and reagents used in this study were of analytical quality and used without additional purification. 35% pure hydrogen peroxide (H_2O_2) was obtained from R & M Chemicals. Sigma Aldrich supplied Poly (Vinylidene Fluoride) (PVDF) with a molecular weight of 534,000 Daltons. Fisher Scientific (M) and Sdn Bhd provided Dimethyl sulfoxide (DMSO). Sodium Dodecyl Sulfate (SDS) with a purity of approximately 95% based on the total alkyl sulfate content and analytical grade methylene blue dye were purchased from Merck, Germany. 18 MΩ·cm resistivity Milli-Q deionised water sourced from potable water was used for all studies, using a PureLab Option-Q system.

2.2 Formation of Fe_3O_4 Nanoparticles/PVDF Macrospheres

Fe_3O_4 nanoparticles were synthesized using a well-established co-precipitation method under inert conditions, as described in our previous work [29]. To prepare the Polyvinylidene Fluoride (PVDF) solution, 10 g of pre-dried PVDF powder was dried in a vacuum oven at 25°C for 5 h. The dried PVDF powder was dissolved in 90 g of Dimethyl Sulfoxide (DMSO) solvent in a beaker, and the temperature was monitored using a sensor tip thermometer submerged in the solution. The blend was sealed with parafilm and agitated at 250 rpm. The mixture was heated from ambient temperature to 60°C at a rate of 10°C/min and held at this temperature for 60 min to obtain a uniform solution. The solution was then cooled to 40°C and allowed to stand overnight under continuous stirring at 150 rpm to minimize the presence of trapped air bubbles. Fe_3O_4 Nanoparticles/PVDF Macrospheres were synthesized using the phase inversion method as described in our previous work [19].

2.3 Morphological Properties of Fe_3O_4 Nanoparticles/PVDF Macrospheres

The structure of the Fe_3O_4 nanoparticle/PVDF macrospheres was examined using a field emission scanning electron microscope (FESEM) in secondary electron mode (LEO SUPRA 50VP, Carl Zeiss Inc.). The macrospheres were frozen in liquid nitrogen for 0.5 minutes and then broken using a razor blade to obtain a cross-sectional view. The samples were gold-coated using a K550X sputter coater (Emitech, UK, for 0.5 minutes to ensure electrical conductivity and avoid surface charging in a vacuum. The macrospheres were analyzed using an electron microscope set at a beam electron voltage of 15.0 kV and the working distance of 13 mm.

2.4 Decolorization of Methylene Blue Dye (MB)

The catalytic efficiency of Fe_3O_4 nanoparticle/PVDF macrospheres was evaluated using methylene blue (MB) as a model dye pollutant and its decolorization was studied using a Fenton-like process. Replication studies were performed to confirm the reliability of these findings. Each trial consisted of glass vials containing 15 mL of a solution with an initial dye concentration of 100 ppm mixed with 5 mL of hydrogen peroxide and stirred gently at 30 rpm to ensure complete mixing. The original dye concentration remained constant at 100 ppm throughout this study. Batch investigations were conducted by adding Fe_3O_4 nanoparticle/PVDF macrospheres and immediately starting the testing process under stirring at 80 rpm at room temperature using a SCILOGEX Analog Tube Rotator (USA). The Fe_3O_4 nanoparticle/PVDF macrosphere dosage ranged from 5 to 15 g/L, and the hydrogen peroxide concentrations varied from 10 to 30 mM. The experimental temperature was maintained at approximately 30°C, while the initial pH was varied between 3 and 7. The Fe_3O_4 nanoparticle/PVDF macrospheres were separated post-reaction using a neodymium boron ferrite (NdBFe) cylindrical magnet with a surface magnetization of approximately 6000G from Ningbo YuXiang E&M Int'1 Co., Ltd. Spectrophotometric measurements were performed using a UV-Vis C-7200UV Peak Instrument (China). Readings were taken at a maximum wavelength of 664 nm initially and after 3 h of testing. The measurements were compared with a preexisting standard calibration curve to determine the concentration of MB.

2.5 Feed-Forward Backpropagation (FFBP) ANN Model Development

An artificial neural network model was built using MATLAB R2015a to predict the decolorization of the MB, with the projected decolorization as the output. The input and goal data were extracted from Microsoft 365 Excel and saved in MATLAB workspace in a horizontal orientation. The methods for neural network type, training function, adaptive learning function, network fitting, data division, plot function, network training, and testing were implemented in MATLAB using the editor tab. This model was used to optimize the number of neurons. A feedforward backpropagation neural network (FFBP NN) was used to develop a model for decolorizing the MB. The model included three input variables: initial pH, catalyst loading, and H_2O_2 dose, and one output variable: the decolorization of the MB, as shown in Figure 1. The FFBP NN model was created to forecast the decolorization of the MB using the artificial neural network (ANN) structure shown in Figure 1. The architecture of the FFBP NN model for the decolorization of the MB is shown in Figure 2, which includes an input layer, a hidden layer, and an output layer. The input layers for the three variables are connected to the hidden layer by designated weights and a tansig transfer function. The hidden layer is linked to the output layer for decolorization of the MB through a specific weight and tansig transfer function. The feedforward neural network uses a backpropagation training method. The feedforward backpropagation method functions based on the idea that outputs are influenced by inputs, weights, biases, and the error derived from the difference between the output and the target, which is then propagated back. The weight and bias were modified until a specific error tolerance or epoch number was achieved.

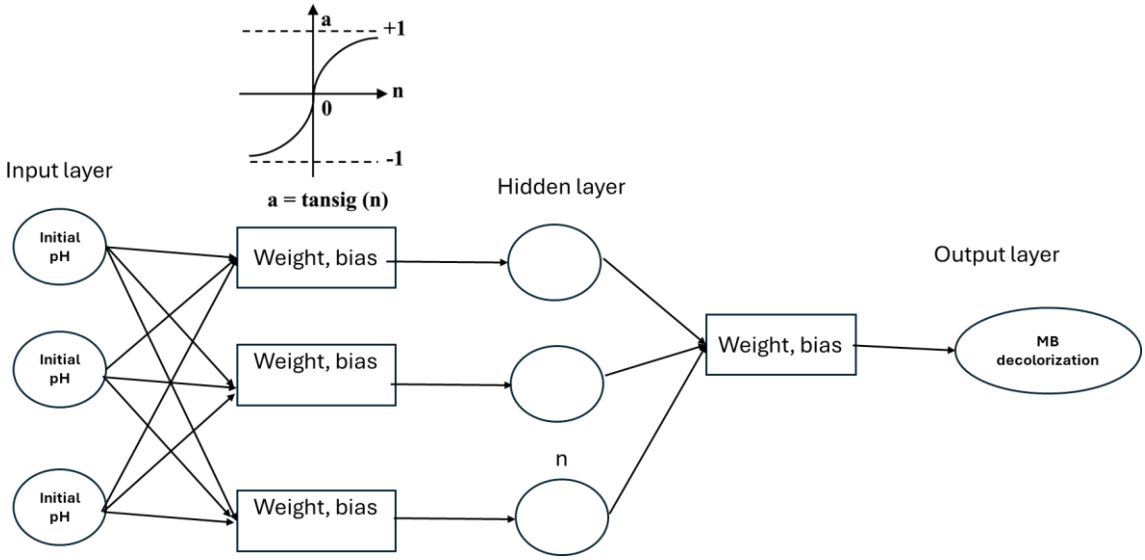

Fig. 1. FFBP ANN model architecture for MB decolorization development

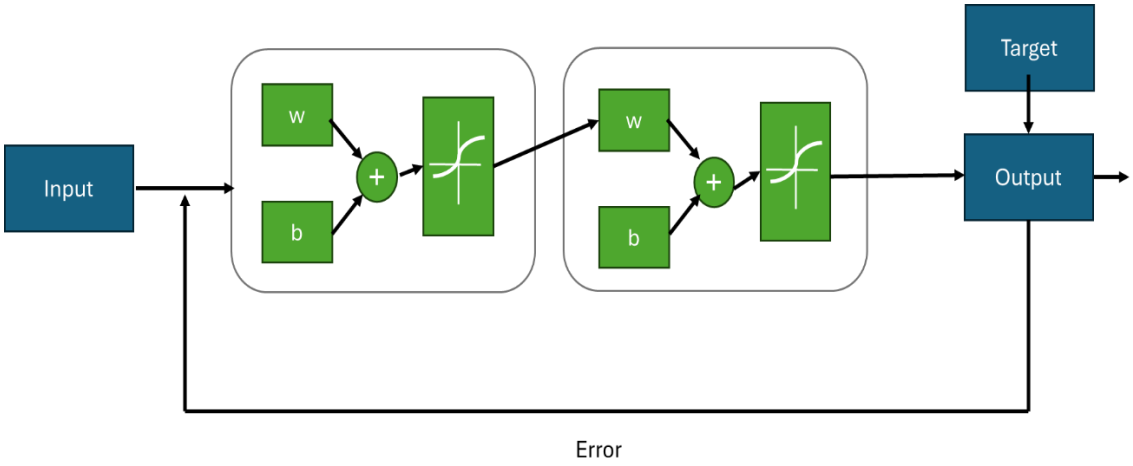

Fig. 2. Mechanism of feed-forward backpropagation neural networks

3. Results and Discussion

3.1 Morphological Properties of the Fe_3O_4 Nanoparticle/PVDF Macrospheres

The SEM images in Figure 3 clearly show the physical characteristics of the Fe_3O_4 nanoparticle/PVDF macrospheres, indicating their potential for environmental remediation, that is, the degradation of pollutants through Fenton-like processes. When viewed at 30x magnification, the outer surface of the macrospheres appeared reasonably smooth with few imperfections. Structural integrity is crucial for preserving the mechanical stability of macrospheres and enabling the selective permeability necessary for successful catalytic interactions [30]. A complicated porous interior structure is visible when the cross-sectional view at 35x magnification. The pores are highly linked, range in size, and resemble an open-cell foam structure. This shape enhances the surface area available for catalytic reactions, which is crucial for the operation of the macrospheres [31]. Examining the sample at 100x magnification reveals variations in the pore size, which significantly impacted the diffusion of reactant molecules inside the macrosphere matrix. The pores in the PVDF matrix were formed by the phase inversion method, which is a commonly used process in polymer science to generate porous structures. This process entails the transition of the polymer from a liquid to a solid phase by a regulated exchange of solvents and non-solvents. The thermodynamics and kinetics of the phase inversion process play crucial roles in shaping the ultimate pore shape [32]. From a thermodynamic perspective, the ability of the polymer to mix with the solvent and the selection of a nonsolvent are important considerations. The extent of phase separation is determined by these factors when a non-solvent is added, which affects the nucleation and development of polymer-rich and polymer-lean phases [33]. From a kinetic point of view, the rate of precipitation of the polymer is influenced by the speed at which the solvent is replaced by a non-solvent. A quick exchange usually leads to a more porous and interconnected structure because of immediate phase separation and rapid polymer precipitation. A slower exchange rate results in gradual phase separation, which may cause the formation of smaller and fewer interconnected pores [34]. The rapid phase inversion process in the Fe_3O_4/PVDF macrospheres was likely facilitated by an optimized solvent and non-solvent system, leading to the formation of an open-cell foam-like structure. This structure provides a high surface area and improves the diffusion efficiency of the reactants. The structural properties enable the efficient diffusion of reactants, such as methylene blue, deep into the macrosphere, ensuring good interaction with catalytic sites made of Fe_3O_4 nanoparticles [18]. The large surface area provided by the interior porous structure improves the interaction between the pollutant molecules and hydroxyl radicals produced in the Fenton-like reaction catalyzed by Fe_3O_4

nanoparticles with hydrogen peroxide (H_2O_2). This chemical process efficiently degrades complex organic compounds, as demonstrated by the fast decomposition of methylene blue.

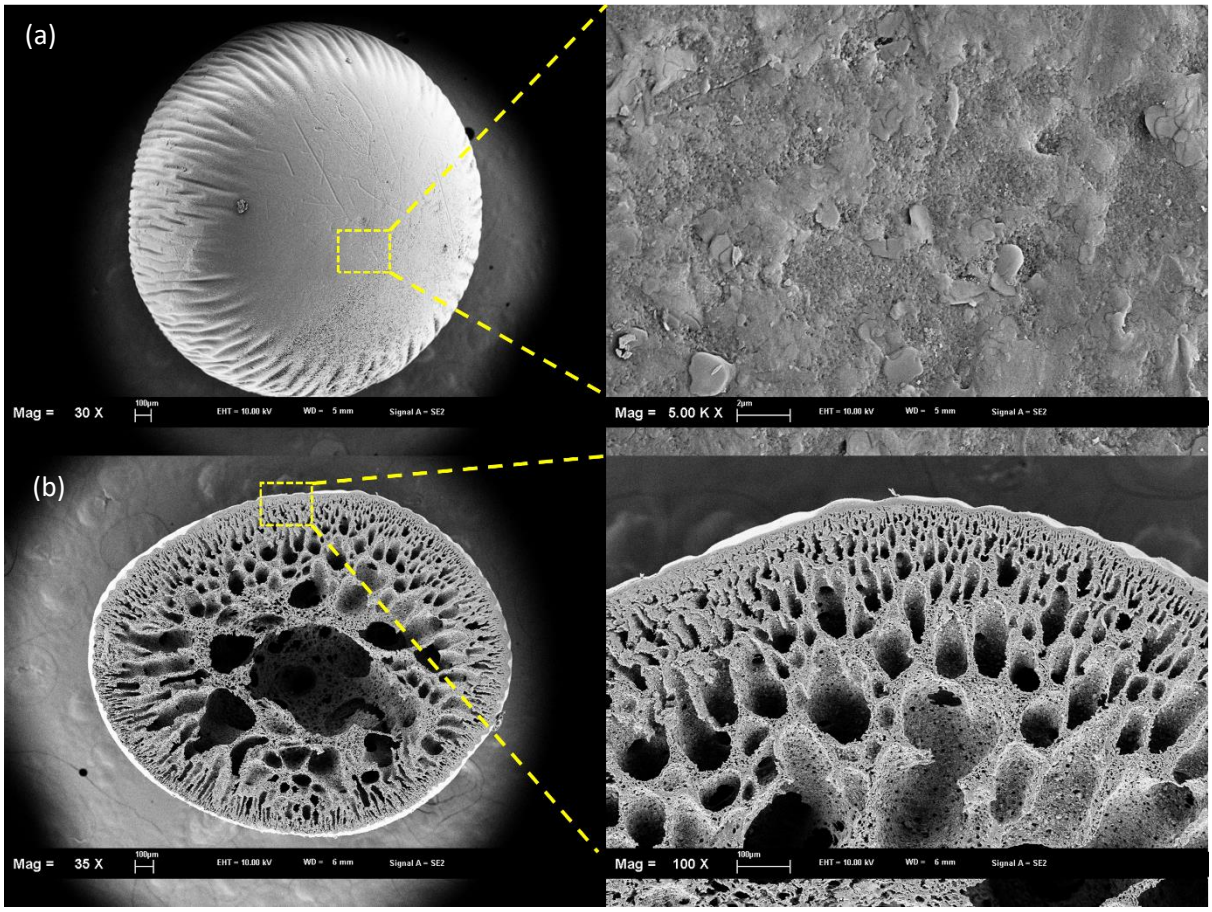

Fig. 3. Scanning Electron Microscopy (SEM) of the Fe_3O_4 nanoparticle/PVDF macrospheres (a) external structure of macrospheres (b) cross-sectional view of the internal structure of macrospheres

3.2 Development of the FFBP ANN Model for Predicting MB Decolorization

In this study, a Feedforward Backpropagation (FFBP) Artificial Neural Network (ANN) model was used to investigate the decolorization of Methylene Blue (MB). This model utilizes distinct architectural and functional elements crucial for effective training and performance, as shown in Table 1. The model uses the Levenberg-Marquardt backpropagation training function, which is known for its effectiveness in minimizing the mean squared error (MSE) as the performance function. The supervised learning model consisted of three layers: an input layer, a hidden layer, and an output layer.

The transfer function of the input layer is defined as a hyperbolic tangent sigmoid function (tansig), which successfully manages the nonlinear properties of the input data. This option simplifies the management of intricate patterns in data that are commonly linked to color-elimination procedures [35]. The model has two transfer functions inside its structure, which improve its capacity to represent nonlinear interactions found in environmental engineering processes. The output layer employs a linear (purelin) transfer function, which is suitable for regression and continuous output applications, such as forecasting the concentration of MB post-treatment with a catalyst. The hidden layer uses a hyperbolic tangent sigmoid transfer function, which is the same as the input layer, to ensure non-linear processing across the network. The model was set up using three neurons in both

the input and hidden layers and one neuron in the output layer to effectively represent the kinetics of MB decolorization. The network completed ten training iterations, indicating the beginning of the study of model suitability or a preliminary phase in model training before a more extended training regimen.

Table 1
Features of the developed FFBP ANN model

Model	Property	Value/remark
ANN	Training function	Levenberg–Marquardt backpropagation
	Performance function	MSE
	Learning	supervised
	Input layer transfer function	Tansig
	Number transfer function used	2
	Output layer transfer function	Purelin
	Hidden layer transfer function	hyperbolic tangent sigmoid (tansig)
	Number of training iterations	10
	Number of input neurons	3
	Number of hidden neurons	3
	Number of output neurons	1

The effectiveness of a Feedforward Backpropagation Artificial Neural Network (FFBP ANN) in predicting the decolorization of Methylene Blue (MB) through the structured experimental approach outlined in Table 2 was assessed. The study was organized based on three variable factors: initial pH (Factor A), catalyst loading (Factor B), and hydrogen peroxide (H_2O_2) dosage (Factor C). The components were varied in 17 experimental runs to assess the predictive ability of the ANN model under various chemical conditions. The experimental matrix was changed in a methodical manner as follows. Factor A was set to pH levels of 3, 5, and 7. Factor B had concentrations of 5, 10, and 15 mg/L. Factor C comprised dosages of 10 mM, 20 mM, and 30 mM. The main goal was to assess and contrast the degree of MB decolorization in the experimental data with the forecasts generated by the FFBP ANN. Data analysis showed that the Artificial Neural Network (ANN) predictions closely matched the experimental results, indicating the model's excellent predictive accuracy. At pH 7, with a catalyst loading of 10 mg/L and H_2O_2 dosage of 30 mM, the ANN model accurately predicted a decolorization percentage of 98.32%, which closely matched the experimentally observed value of 98.25%. The accuracy of the Artificial Neural Network (ANN) model in simulating the complex dynamics of MB decolorization remained consistent across different experimental settings, such as variations in pH and catalyst doses, demonstrating its durability [28].

Table 2
The three-factor experimental response and the value of prediction by the developed FFBP ANN models

	Factor A	Factor B	Factor C	Experimental response	ANN predicted response
Run	A:initial pH	B:Catalyst loading	C:H_2O_2 dosage	MB decolorization	MB decolorization
		mg/L	mM	%	%
1	7	10	30	98.25	98.32
2	5	10	20	94.05	94.06
3	5	5	30	94.26	94.25
4	7	10	10	99.77	99.77
5	5	10	20	94.05	94.06
6	3	15	20	96.45	96.45
7	7	15	20	99.21	99.16
8	5	10	20	94.05	94.06
9	7	5	20	98.37	98.37
10	3	10	30	94.09	94.06
11	5	15	30	95.49	94.06
12	3	10	10	95.11	95.11
13	5	10	20	94.05	94.06
14	5	5	10	96.26	96.26
15	3	5	20	92.68	92.68
16	5	10	20	94.05	94.06
17	5	15	10	97.18	97.18

Figure 4 displays the correlation between the experimentally measured and Artificial Neural Network (ANN)-predicted decolorization percentages of Methylene Blue (MB) under various conditions outlined in the experimental study. The scatter plot illustrates individual data points representing different experimental runs, with each point indicating the percentage of MB decolorization experimentally achieved plotted against the prediction made by the ANN. The linear regression line fitted through the data points, described by the equation $y = 1.0039x - 0.4587$, suggests an almost perfect linear relationship between the observed and predicted values, emphasizing the high accuracy of the ANN model in simulating the outcomes of MB decolorization. The slope of the line, slightly greater than 1, indicates that the ANN model predictions were closely aligned but slightly overestimated the experimental results. This was further confirmed by the high coefficient of determination ($R^2 = 0.9744$), which quantifies the proportion of variance in the observed data that is predictable from the input variables.

The proximity of the R^2 value to 1.0, signifies an excellent fit, highlighting the robustness of the model and its ability to generalize well across the range of experimental conditions tested [36]. This predictive reliability is essential for deploying such models in practical scenarios, where they can guide the optimization of operational parameters in real-time applications for water treatment facilities [27].

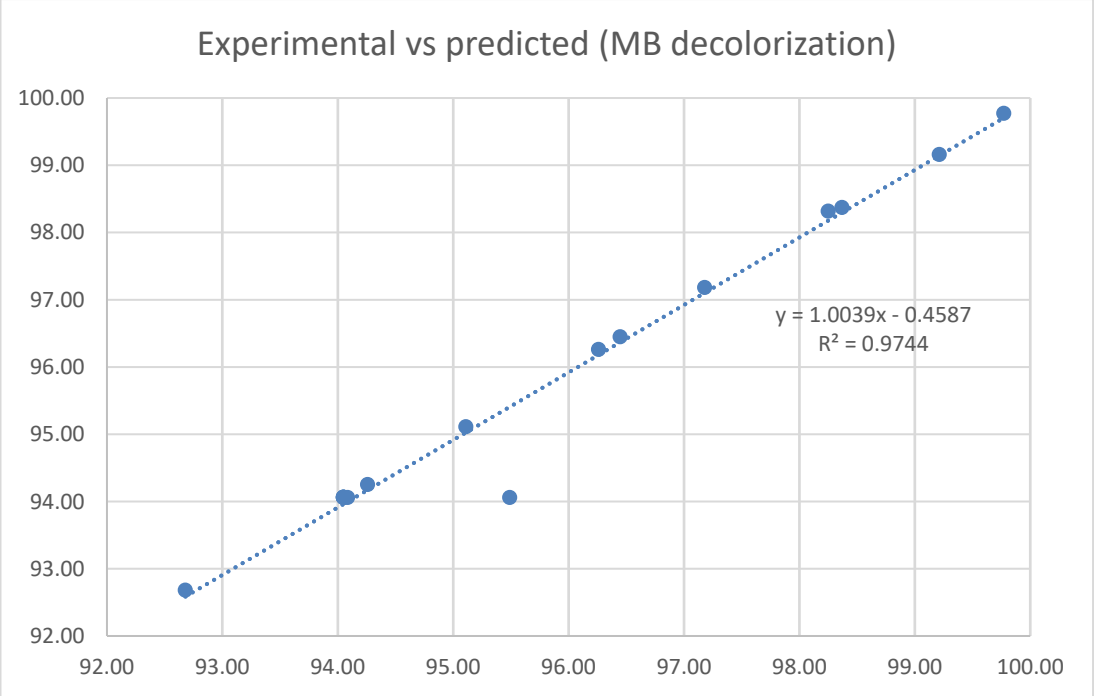

Fig. 4. Comparison between experimental and ANN model-predicted MB decolorization

Figure 5 displays the regression analysis of a feedforward backpropagation Artificial Neural Network (FFBP ANN) used to predict the decolorization of Methylene Blue (MB). This analysis offers a thorough examination of the model's predicted accuracy on various datasets such as training, validation, testing, and the overall dataset. Throughout the training phase, the model showed a strong linear relationship between the predicted and actual decolorization percentages with a correlation value (R) of 0.9786. The alignment between the predictions and the actual data during training indicates that the Artificial Neural Network (ANN) has effectively captured the underlying patterns, as shown by the data points closely following the fitted blue line. During the validation phase, the performance of the model improved, achieving an R-value of 0.99865. This demonstrates a strong generalization ability on unfamiliar data, which is essential for ensuring the model's relevance beyond the training set [37]. The closely clustered data points along the green line validate the capacity of the model to generalize well without overfitting [36]. The regression plot of the testing dataset shows a strong connection with an R-value of 0.99999, as indicated by the red line. The strong correlation between the model predictions and real-world outcomes suggests that the model is reliable and suitable for practical use. This shows that the Artificial Neural Network can effectively forecast MB decolorization in diverse situations, similar to those used for training.

The model demonstrated a strong correlation coefficient of 0.98713 when all data points were considered, as indicated by the gray line. The model demonstrated consistent and reliable performance throughout all the evaluation stages, highlighting its usefulness in mimicking the MB decolorization process.

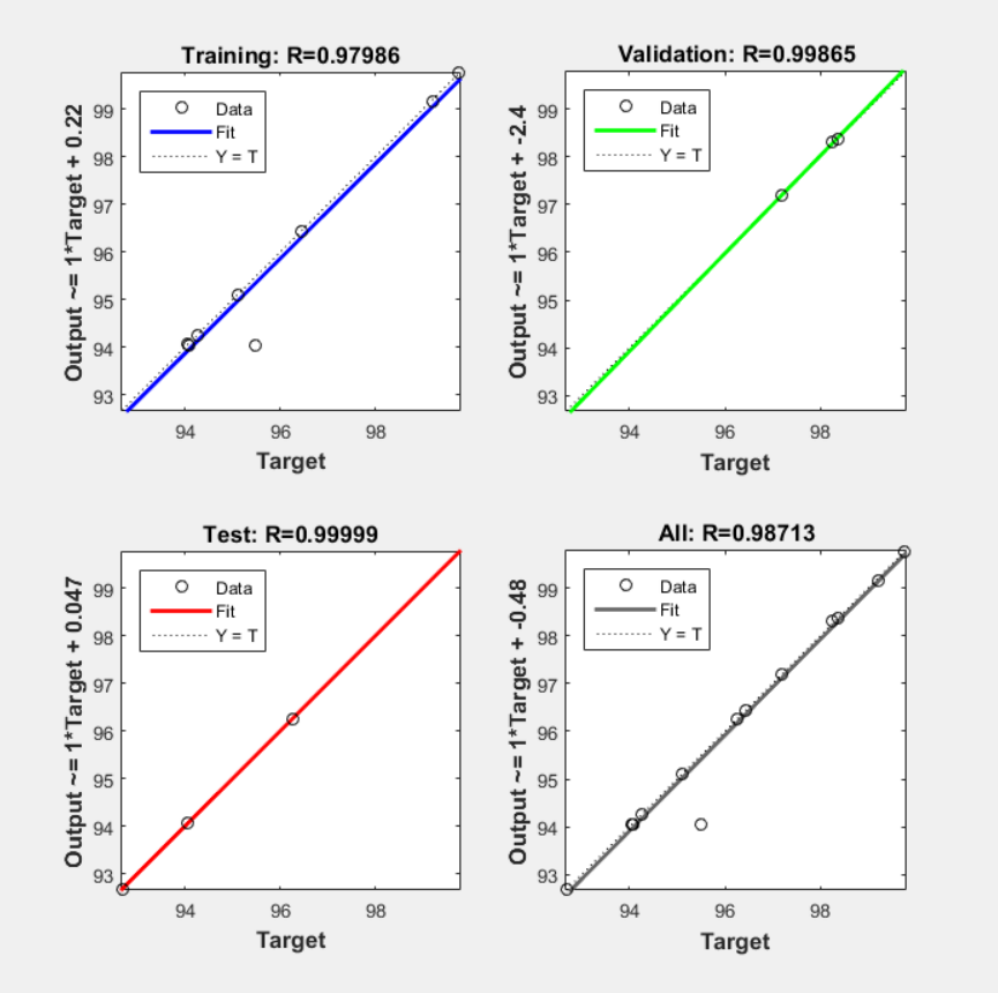

Fig. 5. Regression plot for FFBP ANN model

Table 3 displays the calibration and validation data of a Methylene Blue (MB) decolorization model from ten experimental runs, including the calculated averages for the training, validation, and testing phases. The decolorization model showed incremental performance improvement during the training phase. The initial run achieved a decolorization accuracy of 0.96074, and the subsequent runs indicated modest gains, reaching an accuracy of 0.99996 in the tenth run. The mean accuracy across all training iterations was significantly high, suggesting a strong model training. During the validation phase, the model consistently produced high decolorization accuracies, surpassing 0.98 in all runs, except one. The highest performance was recorded during the fifth run with an accuracy of 0.99999, whereas the lowest was 0.98096 in the second run. The validation accuracy was exceptionally high, indicating the remarkable ability of the model to generalize new data. The testing phase results, which are essential for assessing the practicality of the model, demonstrated strong decolorization accuracies that were largely consistent with the validation phase results. During the testing phase, the accuracy ranged from 0.94749 in the tenth run to 0.99940 in the eighth run. The testing accuracy was slightly lower than the validation accuracy but still good, highlighting the effectiveness of the model in real-world situations. The decrease in accuracy during the tenth testing run may be due to model overfitting or deficiencies in addressing edge situations in the testing dataset [28]. This variation highlights the need to refine the model further to improve its resilience. This model demonstrates remarkable stability in performance compared to other neural network applications in decolorization processes, which often exhibit varying stabilities between runs. This suggests a well-optimized model design [38]. The findings of this study align with the patterns

observed in comparable research utilizing ANN models for optimizing chemical processes. Studies such as that conducted by Nnaji *et al.*, [39] have shown that Artificial Neural Networks (ANNs) can accurately anticipate the results of intricate chemical reactions, such as dye degradation [39]. This model appears to outperform typical benchmarks by consistently achieving high accuracy throughout all stages of modeling, indicating a superior level of optimization that is rarely documented in the literature. Newhart *et al.*, [27] emphasized the importance of precise predictive models in environmental applications to ensure the effectiveness and safety of treatment processes [27].

Table 3
Data calibration and validation of MB decolorization model

Run number	MB decolorization		
	Training	Validation	Testing
1	0.96074	0.99811	0.99689
2	0.96769	0.98096	0.99859
3	0.98555	0.99746	0.99664
4	0.99522	0.99789	0.99248
5	0.99864	0.99999	0.99537
6	0.99970	0.99998	0.99762
7	0.99877	0.99845	0.97413
8	0.99928	0.99989	0.99940
9	0.99304	0.99097	0.99737
10	0.99996	0.96581	0.94749

Figure 6 shows the relationship between the number of iterations and Mean Square Error (MSE) of the Methylene Blue (MB) decolorization model. The graph displays a non-linear trend with an initial decrease in the Mean Squared Error (MSE) from the first to the sixth iteration, followed by a significant rise until the ninth iteration, and a slight stabilization by the tenth iteration. The Mean Squared Error (MSE) decreases steadily from approximately 0.16 in the first iteration to a minimum of approximately 0.02 by the sixth iteration. The reduction in error indicates that the model enhances its accuracy and adapts effectively to the data, demonstrating successful learning and flexibility in its first stages. Between the seventh and ninth iterations, there was a notable increase in the Mean Squared Error (MSE), reaching a peak of approximately 0.14. This increase may indicate overfitting, a situation in which the model begins to focus on insignificant aspects in the training data rather than the essential pattern, resulting in a decline in its ability to perform effectively on new data [40]. By the final iteration, the Mean Squared Error (MSE) stabilizes, suggesting that the model may have reached its learning capacity with the current configuration and data. This trend highlights the importance of continuously checking the model performance over several iterations to prevent overfitting and ensure the model's robustness and accuracy in real-world situations [41]. The observed trends in Mean Squared Error (MSE) over the model iterations suggest a typical pattern of rapid early enhancement followed by a term of stability, which is a common occurrence in machine-learning model training. Khairudin *et al.*, [28] conducted study that revealed similar results to prior studies, showing comparable Mean Squared Error (MSE) patterns in Artificial Neural Network (ANN) models utilized for water treatment procedures. The abrupt increase in Mean Squared Error (MSE) in subsequent rounds is atypical and warrants further investigation [28].

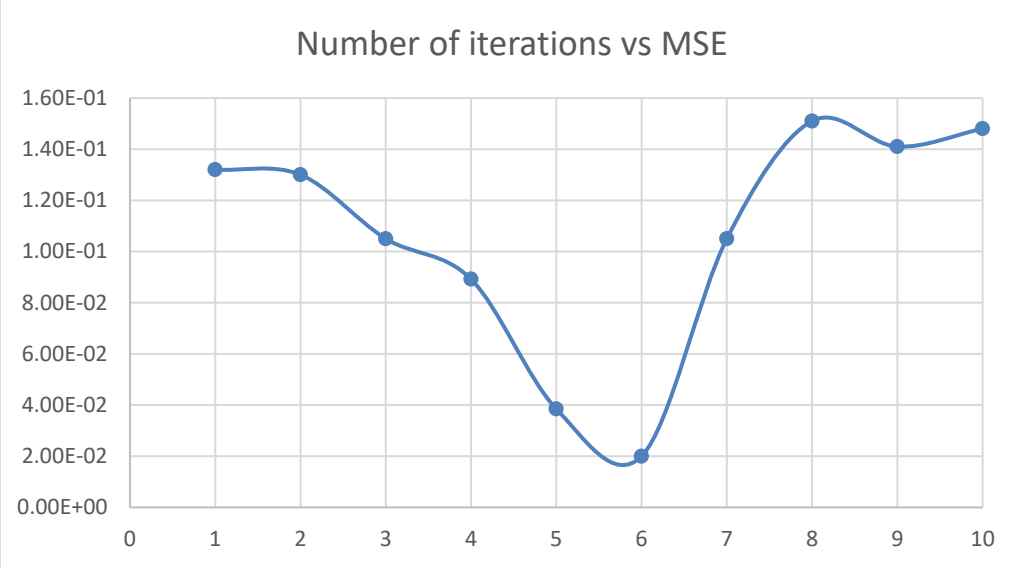

Fig. 6. Iteration of MB decolorization model as a function of Mean Square Error (MSE)

Table 4 displays the performance characteristics of the generated Feedforward Backpropagation Artificial Neural Network (FFBP ANN) model. These indicators are crucial for assessing the precision and efficiency of predictive analytics models. The Mean Square Error (MSE) is 0.0200, indicating the average magnitude of the prediction errors. This value indicates a low error magnitude, which is beneficial for the model performance. The Root Mean Square Error (RMSE) is a crucial statistic derived by taking the square root of the Mean Squared Error (MSE), resulting in a value of 0.1414. The RMSE is valuable as it presents the error size in the same units as the expected result, simplifying its interpretation in real-world scenarios. The RMSE shows that the model's predictions differ from the actual values by approximately 0.1414 on average, confirming the accuracy of the model.

The model's coefficient of determination, R^2, is 0.9744. This statistic quantifies the amount of variability in the dependent variable, which can be explained by independent factors. A high R^2 value indicates that the model explains a large percentage of the variance, showing strong model fit and predictive ability. The correlation coefficient (R) was 0.9871, showing a significant positive association between the observed values and the model predictions. This strong association further confirms the efficacy of the model in precisely capturing and predicting fundamental patterns in the data. The performance metrics of the FFBP ANN model show its resilience and reliability, with strong R^2 and R values indicating that the model can accurately predict fresh data points, validating its usefulness in actual applications. The substantial R^2 and R values meet or beyond standards set by previous scholarly articles, highlighting the model's usefulness in explaining variation and its link with real outcomes. Najah *et al.*, [35] thoroughly explored the necessity of high correlation and determination coefficients when applying neural networks in the environmental and chemical engineering domains. The model's performance not only confirms its existing usefulness but also adds to the overall discussion on enhancing the effectiveness of ANNs for intricate forecasting assignments [35].

Table 4
Performance indicator of the developed FFBP ANN model

Performance indicator of ANN model	Value
Mean Square Error (MSE)	0.0200
Root Mean Square Error (RMSE)	0.1414
R	0.9871
Coefficient of determination (R^2)	0.9744

4. Conclusions

In conclusion, the development and evaluation of a Methylene Blue (MB) decolorization model, implemented through a Feedforward Backpropagation Artificial Neural Network (FFBP ANN), has demonstrated outstanding performance across multiple metrics. The calibration, validation, and testing phases outlined in our study showed a high degree of accuracy, with the model achieving near-perfect scores in the validation phase and maintaining strong performance under testing conditions.

Significant improvements in training performance were evident, as shown by the incremental increase in accuracy from the initial to the final training iterations. The validation results further underscore the model's ability to effectively generalize to new data, which is critical for practical deployment scenarios. Moreover, the testing phase results aligned closely with the validation data, reinforcing the robustness and reliability of the model in real-world applications.

A detailed examination of the model's iterations versus the Mean Square Error (MSE) presents an insightful narrative of the learning dynamics. An initial decrease in MSE indicates efficient learning, whereas a subsequent increase suggests potential overfitting issues, which are then mitigated as the model stabilizes in the latter iterations. This dynamic response emphasizes the necessity of careful iteration management to optimize the model performance.

Furthermore, performance metrics, such as MSE, Root Mean Square Error (RMSE), coefficient of determination (R^2), and correlation coefficient (R), are exceptionally favorable. An MSE of 0.0200 and RMSE of 0.1414 illustrate the precision of the model in predicting the decolorization of MB. The high R^2 value of 0.9744, along with a correlation coefficient of 0.9871, demonstrates the accuracy of the model and its capability to explain a significant proportion of the variance in decolorization outcomes from the input variables.

These results collectively affirm that the ANN model is not only theoretically sound, but also practically viable for addressing challenges in water treatment processes, specifically in the decolorization of industrial dyes such as Methylene Blue. The findings of this study provide valuable insights into the field of environmental engineering and have substantial implications for the design and implementation of more efficient water-treatment solutions. The successful application of such models could lead to significant advancements in the sustainability and effectiveness of water purification technologies, which are crucial for both environmental protection and resource management in industrial applications.

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