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Modeling of Dispersed Red 17 Dye Removal from an Aqueous Solution Using Artificial Neural Network

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ABSTRACT

A significant amount of hazardous compounds has leaked into the environment due to the widespread usage of organic dyes, and it is essential that these dangerous contaminants be removed in a sustainable way. This study used varying amounts of H_2O_2 (0, 0.5, 1.5, 3, and 5) mM/L to extract the dye from the aqueous solution. Furthermore, concentrations of 0.4, 1, 1.7, and 2.3 mM/L of Fe^{+2} as $FeSO_4 \cdot 7H_2O$ were also utilized. Batch Advanced Oxidation Process (AOP) was carried out under various working conditions, including: contact time (5–60 min), mixing speed (100–300 rpm), and UV light intensity (0–40 W). Utilizing experimental data, the AOP efficiency of Dispersed Red 17 Dye was calculated. Genetic Cascade-forward Neural Network (GCNN) was employed as a machine-learning tool to forecast the oxidation efficiency and the amount of dye that would be removed from the aqueous solution, specifically Dispersed Red 17. When compared to experimental data, the best model had an R^2 correlation value of 0.955. The findings of the importance analysis showed that the studied parameters affected the discoloration efficiency with order of: H_2O_2, UV, Fe^{+2}, mixing speed, and contact time. The obtained results demonstrated the effectiveness of GCNN as a novel approach in forecasting the AOP efficiency of Dispersed Red 17 Dye.

Keywords: modeling, wastewater, AOP, dye removal, artificial neural, GCNN.

INTRODUCTION

The adverse impact of climate change on water availability has increasingly ignited interest on wastewater reclamation and enhanced the efforts to explore innovative ways to save water resources for next generations [1, 2]. The removal of hazardous dyes from industrial wastewater is an increasingly critical concern in environmental science and engineering. Dispersed Red 17 Dye, a common organic dye used in industries such as textiles and dyeing due to high compatibility with hydrophobic fiber [3], poses a significant threat to both the environment and human health unless effectively eliminated from aqueous solutions [4, 5]. Around (280,000 tons/year) of dyes are being discharged into wastewater streams [4, 5]. In response to this challenge, Fenton process has been employed successfully to remove various refractory substances from wastewater [5, 6]. A well-known advanced oxidation process (AOP) is powerful oxidative for the removal of recalcitrant organic contaminants from water and wastewater, the Fenton process is a efficient and versatile technique. The Fenton technique offers a glimmer of hope in an era where environmental pollution is becoming an increasingly pressing globally concern. It is depending on a simple chemical process that generates hydroxyl radicals (OH*), which is one of the most powerful oxidative species recognized to technology. Numerous organic substances, such as, dyes, can be efficiently oxidized by these radicals converting them to harmless and non-toxic to the ecosystem. Because of its effectiveness in breaking down prolonged pollutants, which includes industrials dyes, pharmaceutical residues and new toxins, the Fenton process is becoming more and more famous and useful in the fight for eco-friendly water and wastewater treatment [2, 7]. Despite the high performance of AOP, the main drawback, however, is the elevated cost of application due to using chemical reagents in this process. The use of hydrogen peroxide (H_2O_2) and ultraviolet (UV) light in large-scale applications of water wastewater treatment can indeed raise environmental and safety considerations. For that reason, it is important to carefully assess and mitigate the potential risks associated with these technologies, even though H_2O_2 has been reported as a green oxidant [8]. The efficiency of AOP was investigated through experimental work and systematic analysis of the role of the intensity of applied UV, mixing speed, H_2O_2 doses, Fe^{+2} concentration, and contact time.

PROPOSED GENETIC CASCADE-FORWARD NEURAL NETWORK

In order to achieve feasible and cost-effective ways to investigate the performance of AOP, researchers have turned to advanced technologies, particularly integrated artificial neural networks (ANNs) with genetic algorithms (GA), as a promising approach for modeling and optimizing the removal of these dyes from water [9]. The application of genetic cascade-forward neural network (GCNN) in wastewater treatment represents a cutting-edge approach to optimizing and enhancing the efficiency of water purification processes [10]. GCNN is a novel architecture that influences the power of genetic algorithms to evolve and optimize neural network structures, allowing for the automatic discovery of complex and efficient network architectures (Figure 1). This approach holds promise for addressing the challenges of feature selection, network design, and hyperparameter tuning, which are often labor-intensive and time-consuming processes in traditional neural network development [11]. By integrating the principles of evolution and selection, GCNNs have the potential to revolutionize the field, providing efficient and customized solutions for a wide range of tasks, from pattern recognition to predictive modeling, and ultimately advancing the frontiers of artificial intelligence. The GCNN is adaptive for the studied application, where the inputs were considered as: H_2O_2, UV, Fe^{+2}, mixing speed and contact time, and the output was assigned for removal efficiency. In addition, the numbers of utilized hidden neurons, connection weights and layer can be considered suitable according to the proposed method of GCNN. Such numbers are varied and may not be sufficient for other traditional ANN models. By employing GCNN-based modeling, this study sought to contribute to more effective and sustainable solutions for treating industrial wastewater, thereby safeguarding the environment and human well-being. GCNN has obtained the outcomes that can provide insight overview for the case of cost-effectiveness after considering all accountable cost requirements. Moreover, this model can be adapted or expanded by considering the required inputs and output, then, training the new model and – consequently – testing the trained model.

Importance equation

The importance equation of a neural network-based approach is a fundamental concept in understanding the inner workings and decision-making processes of these complex machine-learning models. This equation helps reveal the significance of each input feature in the output of the neural network, allowing researchers to identify which features have the most substantial influence on the model's predictions. By assigning importance scores to input features, the equation aids in feature selection, model interpretability, and fine-tuning, enabling data scientists and researchers to focus on the most relevant factors. This knowledge not only enhances the model's performance but also provides valuable insights into the relationships between input variables, ultimately advancing scientists understanding of the neural network's decision-making logic. The importance equation, often computed through techniques like feature importance scores or gradient-based methods, plays a crucial role in various applications and a key component in optimizing the efficiency and accuracy of neural network models. The importance equation that used in this study (Eq. 1) was derived from in some previous publications for the employed cascade-forward neural network [12]. The effect of each variable in the removal process was isolated by eliminating the redundant parameters and maintaining the parameters of a certain input. In other words, these are attained by implementing equation (1).

$$I_j = \frac{\sum_{m=1}^{m=N^h}((\left|w_{jm}^{ih}+w_{jn}^{io}\right|/\sum_{k=1}^{k=N^i}\left|w_{km}^{ih}+w_{kn}^{io}\right|)\times\left|w_{mn}^{ho}+w_{kn}^{io}\right|)}{\sum_{k=1}^{k=N^i}\{\sum_{m=1}^{m=N^h}(\left|w_{km}^{ih}+w_{jn}^{io}\right|/\sum_{k=1}^{k=N^i}\left|w_{km}^{ih}+w_{kn}^{io}\right|)\times\left|w_{mn}^{ho}+w_{kn}^{io}\right|\}} \quad (1)$$

where: N^i and N^h are the numbers of input and hidden neurons, respectively; *w's* are connection weights; superscripts '*i*', '*h*', and '*o*' denote input, hidden, and output layers; subscripts '*k*','*m*', and '*n*' denote input, hidden, and output neurons; and I_j is the relative importance of the j^{th} input variable on output variable [12].

This research aimed to explore the application of GCNNs as a powerful tool in the modeling of Dispersed Red 17 Dye removal, offering insights into the intricacies of this removal process and the potential for improving its efficiency. The only drawback associated with this study is that it has a limitation of requiring additional memory size and additional computations for the connection weights between the inputs and output. However, this point can be sorted out by simply employing a computer machine with sufficient or high characteristics. Moreover, in future it can be suggested that other optimization methods can be applied instead of genetic algorithm such as Red Fox optimization (RFO) and Polar Bear optimization (PBO).

MATERIALS AND METHODS

A series of experimental work was done to investigate the effect of hydrogen peroxide (H_2O_2), ferrous sulfide heptahydrate ($FeSO_4.7H_2O$), UV light, contact time and mixing speed on removal efficiency of Disperse red 17 dye ($C_{17}H_{20}N_4O_4$). The concentrations of H_2O_2 were (0, 0.5, 1.5, 3, and 5) mM/L while the concentrations of $FeSO_4.7H_2O$ were (0, 0.4, 1, 1.7, and 2.3) mM/L. Three different intensities of UV light were applied (0, 20, and 40) Watt to enhance the AOP process. Different mixing speed was also applied (100, 200, and 300 rpm) to further improve the contact between chemicals and dye. The role of contact time was also investigated in this study by measuring the removal efficiency after a wide range of time (5,7, 10, 15, 20, 30, 35, 60) minute. The residual dye in solution was detected using UV spectrophotometer at wavelength of 464 nm. For the purpose of comparison, the GCNN has a great advantage over classical backpropagation neural network and cascade-forward neural network. That is, it is not deceived by the local error problem during the training phase. Conversely, both classical backpropagation and cascade-forward neural networks can be tricked by such problem. This is due to the optimization ability of GA in overcoming the problems of local errors and go efficiently toward the global error.

Fitness function

The fitness function of the proposed GCNN approach considers obtaining the minimum error between the targets and outputs of the cascade-forward neural network. It basically produces the investigated weights that provide minimum error value. Thus, the fitness function can be represented by the following equation (Eq.2).

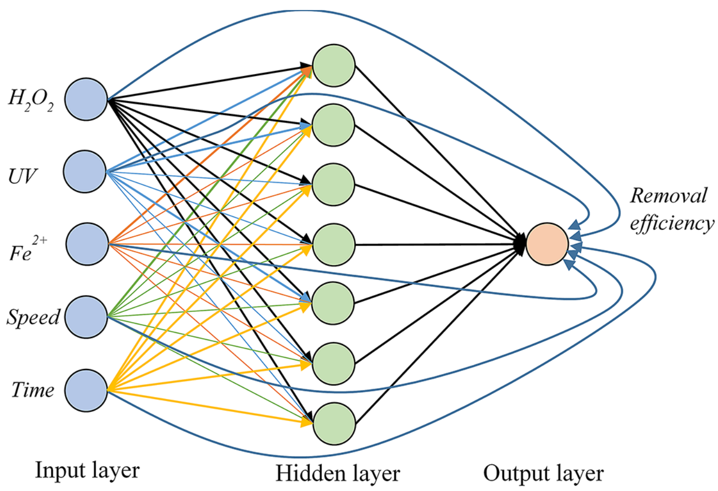

Figure 1. Suggested cascade-forward neural network for predicting the output of removal efficiency from the inputs of H_2O_2, UV, Fe^{+2}, mixing speed, and contact time

$$E(\mathrm{W}) = \frac{1}{S}\sum_{q=1}^{S}\left|T_q - Y_q\right| \quad (2)$$

where: $E(W)$ is the fitness function of the genetic algorithm and it represents the error function of all cascade-forward neural network weights; W, S is the number of available training vectors, T_q is a provided target for q^{th} training vector and Y_q is a cascade-forward neural network output for the same q^{th} training vector.

Other genetic algorithm factors for the proposed GCNN were set as follows: population size (number of utilized chromosomes in each generation) of 200, fitness scaling of type top (considering the top evaluated fitness values), selection of type stochastic uniform, cross-over of type scattered, mutation of type adaptive feasible and stopping criteria for the value fitness limit of 0.177. The produced values of weights were used to test or predict the GCNN, but this time by using the testing vectors. The principles of the testing procedure of the cascade-forward neural network with its final weights can be investigated in previous publications [12, 13].

Test algorithm

GCNN is developed by training its weights according to the genetic algorithm. It is validated by applying the obtained weights in the testing phase, which shows valuable outcomes. A testing process is carried out to assess the correctness of the neural network after the training phase. It has one phase, the same as the feed forward stage of the training algorithm. Neither input data analysis nor output enhancements are being carried out at this time. The main equations used in this case are presented below [11]:

$$z\_in_j = v_{0j} + \sum_{i=1}^{n} x_i v_{ij} \quad (3)$$

$$z_j = f(z\_in_j) \quad (4)$$

$$y\_in_k = w_{0k} + \sum_{j=1}^{p} z_j w_{jk} + \sum_{i=1}^{n} x_i vw_{ik} \quad (5)$$

$$y_k = f(y\_in_k) \quad (6)$$

where: Xi represents the inputs (i = 1,2,3,…, n), vij stands for the connection weights between the input and hidden neurons, Zj is the function calculations of hidden neurons, y_in_k denotes the input calculations of each output neuron (k = 1,2,3,…, m), w_{0k} represents the connection weights between the bias and output neurons, w_{jk} are the connection weights between the hidden and output neurons, vw_{ik} represents the additional connections between the input and output neurons in the central feature network (CFN), and y_k are the function calculations of output neurons.

RESULTS AND DISCUSSIONS

The results of the study are crucial in understanding the potential of the proposed GCNN innovative optimization approach. The investigation included various factors affecting the removal process, such as H_2O_2 concentration, $FeSO_4.7H_2O$ concentration, intensity of UV light, contact time and mixing speed providing valuable insights into the intricate dynamics of the system. Furthermore, the study discussed the practical implications of the ANN-based modeling, highlighting its potential for real-world applications in water treatment and environmental protection. The discussion of the results highlighted several key points:

Predictive accuracy

A robust correlation (0.955) has been observed between the anticipated and experimental removal efficiency, as illustrated in Figure 2. The results of the study probably show that the GCNN model has a high level of predicting accuracy. This indicates that the model can accurately predict how well the dye removal method will work in various scenarios. This is an important point since it shows that GCNNs may be able to provide an accurate tool for assessing the removal effectiveness of Disperse red 17 dye without the need for lengthy and laborious tests.

Influence of input variables on dye discoloration

The relative significance of several input variables that affect the dye removal process is clarified by the importance analysis results. Using this information, one can determine which variables most significantly affect the removal efficiency.

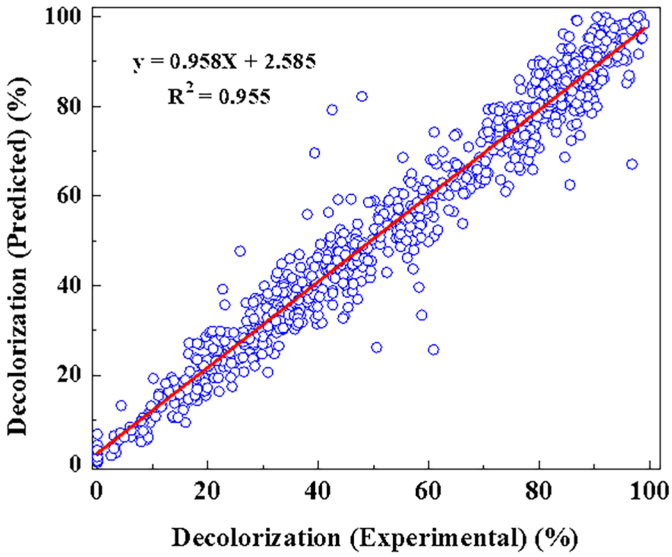

Figure 2. The correlation between predicted and experimental removal efficiency

Gaining insight into these factors facilitates improved process control and optimization.

The influence of H_2O_2

Table 1 demonstrates that H_2O_2 had a greater influence on the dye removal efficacy compared to the other parameters, making it the most significant parameter. Additionally, as seen in Figures (3a through 3e), a strong correlation was examined between the experimental data and the predicted outputs from the GCNN output at different H_2O_2 concentrations (i.e., 0, 0.5, 1.5, 3, and 5 mM/L). Although the importance analysis showed that H_2O_2 was crucial to remove the dye from wastewater, the removal efficiency increased by only 5%, from 83% to 88%, when the dose of H_2O_2 was increased by ten times from 0.5 mM/L to 5 mM/L), it is clear that the concentration of H_2O_2 alone has no obvious effect. This finding is in agreement with previous studies [7, 14]. It is commonly recognized that a rise in H_2O_2 concentration causes a greater concentration of $HO^{\cdot}$ radicals, which are what cause the mineralization process. Hydrogen peroxide excess, on the other hand, decreases the catalytic activity because it promotes the interaction of $HO^{\cdot}$ with peroxide, which lowers the quantity of accessible radicals and produces the scavenger effect. When there is an excess of H_2O_2 in the solution, hydrogen peroxide breaks down to generate water and oxygen (an unproductive process) [15].

Table 1. The importance percentages of studied Input parameters

Variable	Importance (%)
H_2O_2	37.01
UV	21.95
Fe^{2+}	18.03
Speed	16.11
Time	6.90
Total (%)	100

The impact of UV

Three UV power levels (0, 20, and 40 W) were used to increase the effectiveness of dye removal. Figures 4a through 4c illustrate the influence of UV on dye discoloration. From experimental results and GCNN output regarding the UV influence, it can be concluded that the more irradiation may enhance dyes discoloration reactions and lessen their quantity in aqueous solutions [16].

The influence of Fe^{+2}

In water treatment research, the impact of ferrous iron (Fe^{+2}) on wastewater dye removal is an important factor. Through a variety of methods, ferrous iron can be extremely important in the elimination of dyes. Coagulation is a popular technique in which Fe^{+2} functions as a coagulant to destabilize colloidal particles and promote their aggregation. Larger flocs that are easier to separate from the water and transport the dye molecules with them are formed as a result. Ferrous

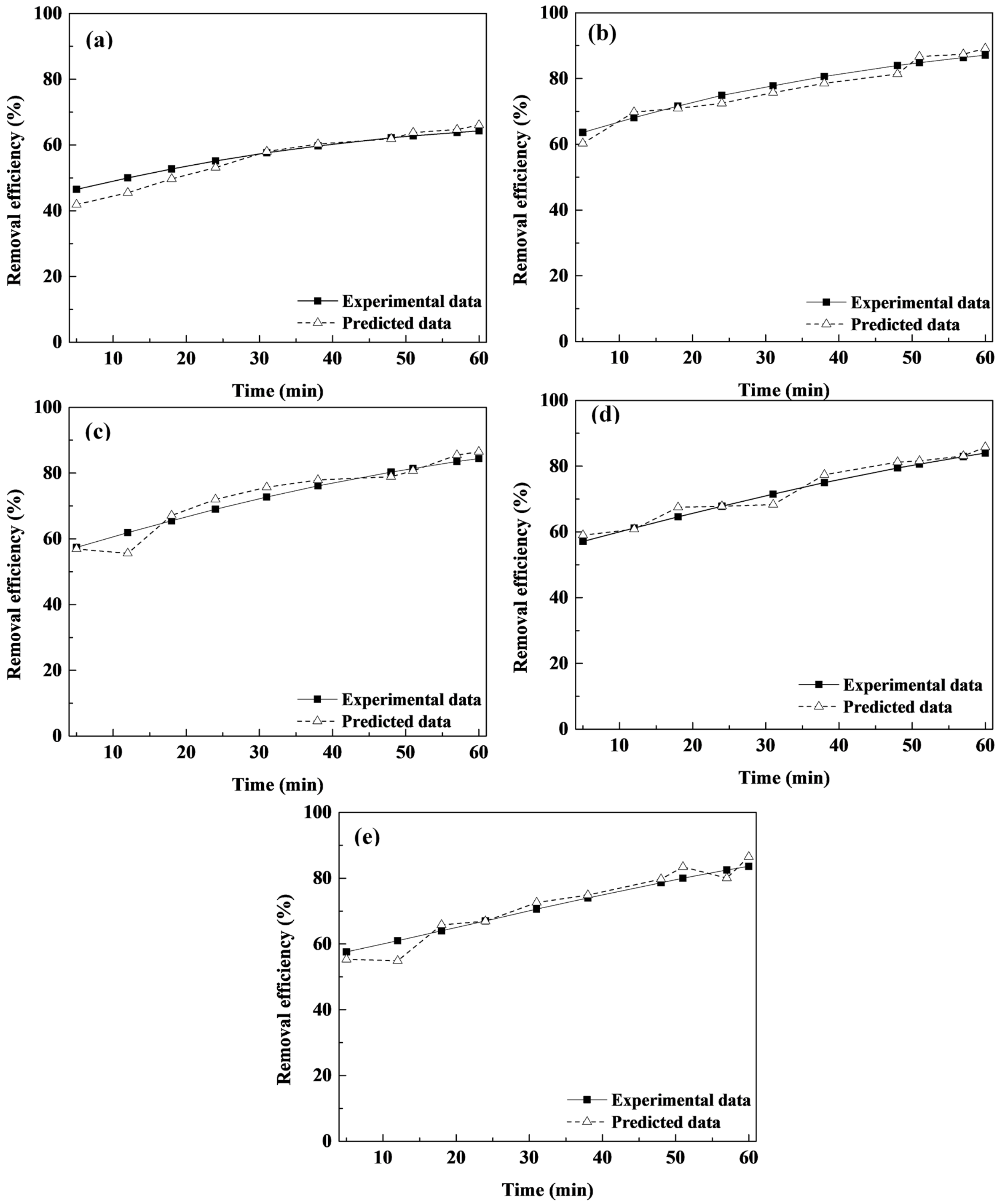

Figure 3. Experimental results and predicted output from GCNN at different H_2O_2 concentrations (a) 0, (b) 0.5, (c) 1.5, (d) 3, and (e) 5 mM/L

iron can also take part in redox processes, which may result in the reduction of certain color molecules. The dye may change into a less soluble or more readily removed form as a result of this decrease. Nevertheless, the kind of dye, the wastewater pH, and the particular treatment method used can all affect how well Fe^{+2} removes dye. Figure (5a through 5e) illustrates the effect of Fe^{+2} dosage on the removal effectiveness of Dispersed Red 17 Dye was examined by applying various doses (0, 0.4, 1, 1.65, and 2.33) mM/L. As the dose of Fe^{+2} increased to 1 mM/L.

By the time the Fe^{+2} dose reached 1 mM/L, the discoloration efficiency had significantly improved. However, the efficacy of dye removal was not significantly affected by the increased

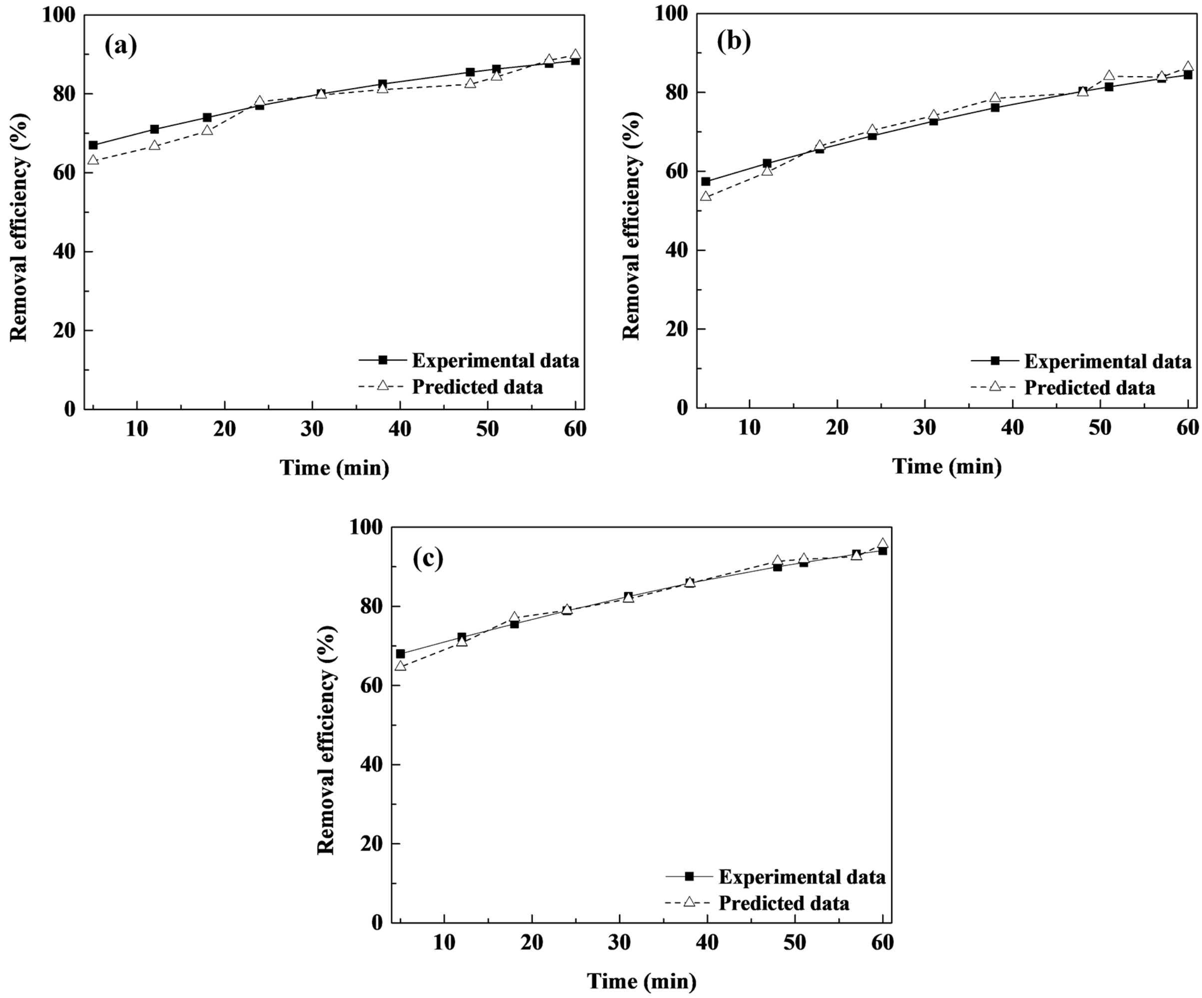

Figure 4. Experimental results and predicted output from GCNN at different speeds UV intensities (a) 0, (b) 20, and (c) 40 W

Fe^{+2} concentration. This suggests that the optimal concentration of Fe^{+2} was 1 mM/L and that Fe^{+2} levels above that have no beneficial effects. The results of other published research that indicated that the ideal concentration of Fe^{+2} to eliminate dyes from wastewater was approximately 1 mM/L are consistent with the conducted study [17].

The role of mixing speed

The impact of mixing speed on dye removal efficiency is a significant factor in many water treatment processes and wastewater treatment systems. The rate at which a dye reacts with oxidants is dependent on the degree of mixing. The impact of various mixing speeds (100, 150, 200, 250, and 300 rpm) on dye removal efficiency is displayed in Figures 6a through 6e. It is evident that 150 rpm was the optimum mixing speed to achieve higher discoloration efficiency. Incomplete dispersion of the dye molecules, which reduces their contact with the treatment chemicals, can result in lower dye removal efficiency. Conversely, very vigorous mixing could reduce the efficiency of removal by obstructing the oxidation process [18, 19].

The influence of time

An important consideration in the treatment of wastewater and water is the effect of contact time on dye removal efficiency. The length of time that solution is exposed to a treatment agent directly affects how well dyes are removed. The longer contact times generally provide dye molecules the more chances to interact with oxidants, increasing the removal effectiveness of the dye. Beyond a certain point, though, an unnecessarily long contact time may not yield a discernible improvement in removal efficiency and may even be impracticable. Therefore, determining the ideal contact time is essential to achieving a balance between effective

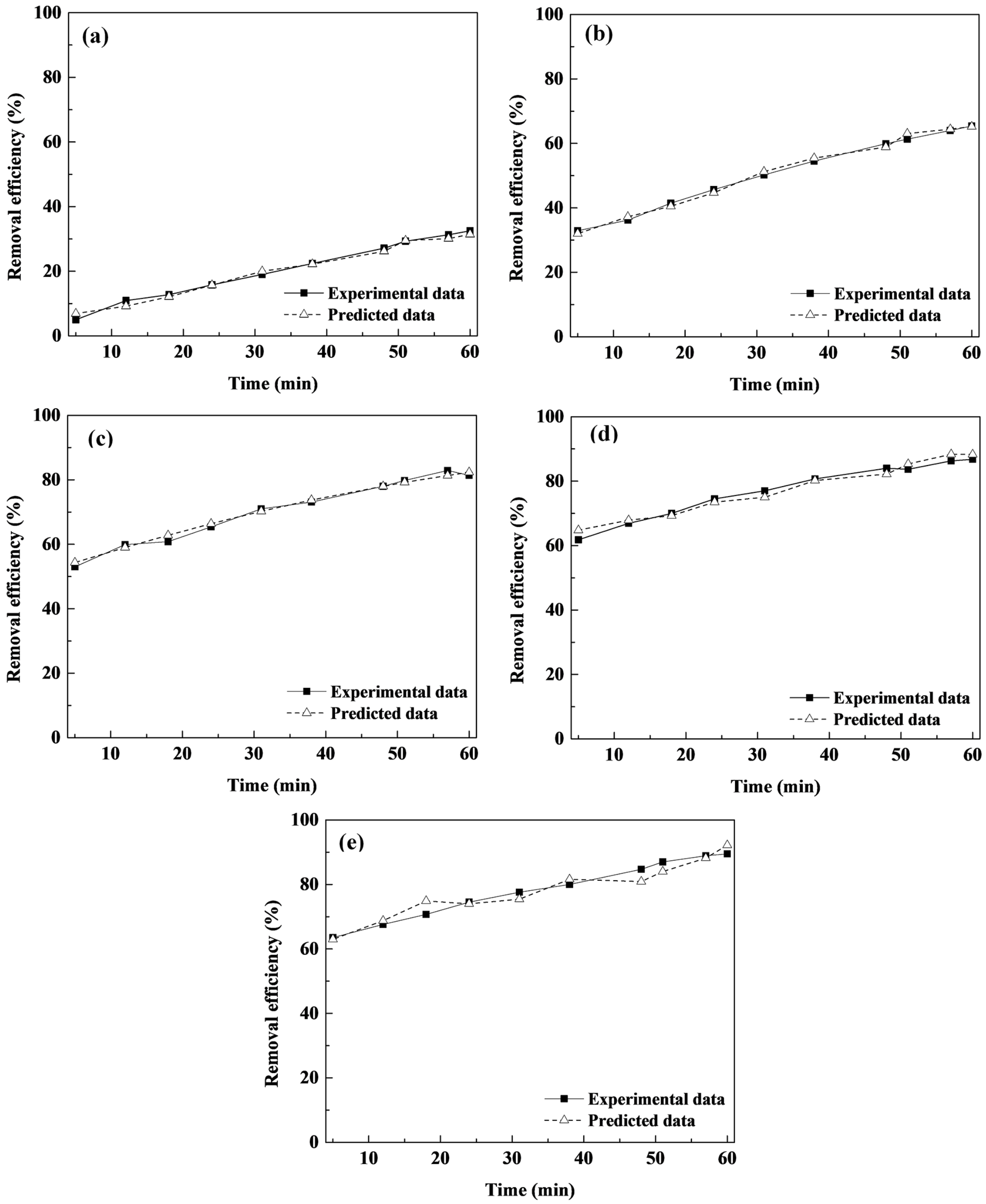

Figure 5. Experimental results and predicted output from GCNN at different Fe^{2+} concentrations (a) 0, (b) 0.4, (c) 1, (d) 1.65, and (e) 2.33 mM/L

dye removal and treatment system practicality. Over time, the discoloration of Dispersed Red 17 Dye improved significantly for all applied conditions. However, after 60 minutes of interaction time, this improvement was not significant. This result demonstrates that extending the duration of contact beyond sixty minutes has no positive effect on removal effectiveness. However, it has been noted that the ideal duration of contact for eliminating certain dyes was less than what was found in this investigation, suggesting that numerous factors, including temperature, pH, and kind of oxidant, influence the discoloration of dye [14, 18].

Environmental and industrial implications

Critical insights into the possibilities of this technology in water treatment and environmental remediation were provided by the findings of this work on the modeling of Dispersed Red 17 Dye removal using GCNNs. They showed how accurate the model is, how well it can highlight different

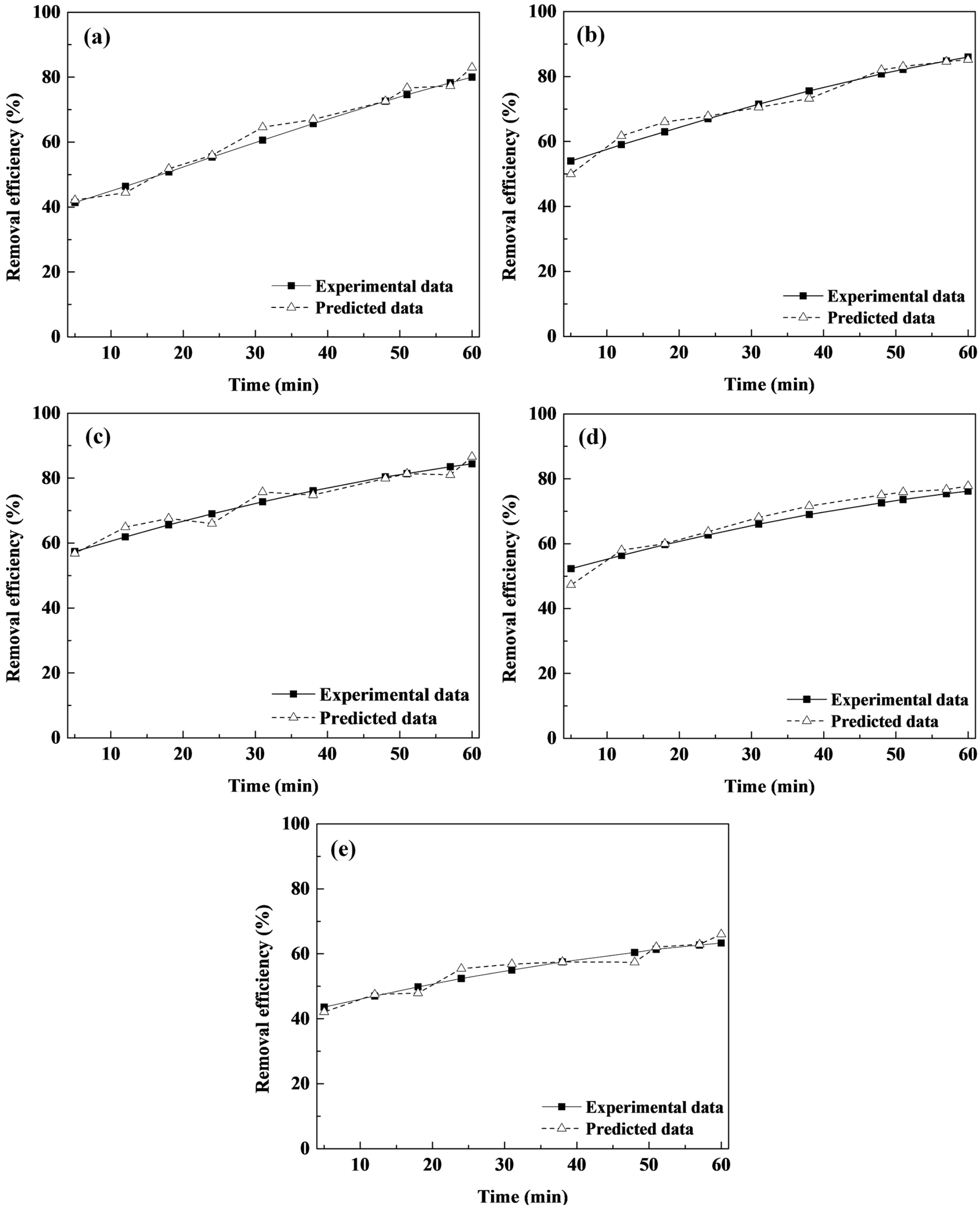

Figure 6. Experimental results and predicted output from GCNN at different speeds (a)100, (b) 150, (c) 200, (d) 250, and (e) 300 RPM

elements, and how useful it is in solving real-world problems. The contribution of this study was to evaluate the efficacy of AOP in a safe, ecologically friendly, practicable, and cost-effective manner.

CONCLUSIONS

The obtained results show that the GCNNs strategy may be successfully used to forecast and maximize the removal efficiency of this hazardous organic dye. The GCNN approach was found to have remarkable prediction accuracy, making it a viable tool for dealing with dye removal issues. The study elucidated the significance of every parameter under investigation and demonstrated that H_2O_2 exerted the greatest influence on the dye removal efficacy from solution. The results of this study established the way for improved and effective approaches to managing dye pollution, which will have a substantial impact on environmental sustainability and water quality management.

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