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Research Article

Applying an Artificial Neural Network to Predict the Mechanical Properties of Epoxy Resin with Graphite Additive After Water Absorption

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ABSTRACT

The present study utilized an artificial neural network (ANN) model to anticipate Barcol hardness, impact strength, and heat deflection temperature data for epoxy resin specimens with varying weight percentages of graphite additive exposed in different types of water. A feedforward backpropagation algorithm was used for predictive modeling with two input parameters: the weight percentage of the graphite additive (0, 5, 10, 15, and 25 wt.%) and the type of water used (dry specimen, potable water, distilled water, alkaline solution, and acidic solution). Experimental test data for mechanical properties were used to train the ANN model. The network was validated by comparing the predicted outputs with experimental data and by evaluating performance metrics. The results conclude that the ANN model is a practical and accurate approach for rapidly predicting mechanical performance and can be considered a substitute for traditional procedures used to characterize composite materials through experimental methods. Among the two input parameters, the weight percentage of the graphite additive was the most essential input parameter used to predict the mechanical properties of composites. Besides, the key findings of this work can also be a reference for the engineering practice of composite materials under mechanical and moisture environments.

1. Introduction

Composite materials, known for their superior mechanical properties and lightweight characteristics, have become indispensable in modern engineering applications. They are widely used across industries such as aerospace, automotive, construction, and marine engineering. However, the design and optimization of composite materials remain challenging due to their complex and heterogeneous nature, where properties depend on various factors such as constituent materials, manufacturing processes, and environmental conditions. Traditional methods for predicting the mechanical and physical properties of composites often involve extensive experimental testing, which is time-consuming, labor-intensive, and costly. As a result, there is a growing need for advanced computational techniques to accurately model and predict the behavior of composites under different conditions. Artificial neural networks (ANNs) have emerged as a powerful tool for addressing these challenges. ANNs are computational models inspired by the human brain, capable of learning complex patterns and relationships

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from data. They have demonstrated remarkable success in various scientific and engineering fields due to their ability to model nonlinear systems, handle large datasets, and generalize predictions for new conditions.

Recently, numerous studies have focused on applying artificial neural networks (ANNs) in the characterization of composite materials. Researchers have explored various ANN-based techniques for predicting mechanical properties, damage detection, and optimizing material structures. Zenzen et al. [1] proposed a modified damage indicator and an ANN model to estimate the location and size of damage in composite structures. Their approach effectively identified damaged elements with reduced computational time. Similarly, Tan et al. [2] developed a procedure for detecting damage in a composite slab-on-girder bridge using vibration characteristics and ANN. Their results confirmed its feasibility in damage detection and quantification. Khatir et al. [3] introduced an improved artificial neural network using an arithmetic optimization algorithm for damage assessment in functionally graded material (FGM) composite plates, achieving high precision in predicting damaged elements. Mardanshahi et al. [4] employed guided wave propagation and artificial intelligence to develop an intelligent model for detecting and classifying matrix cracking in glass/epoxy composites using data from Lamb wave propagation. In mechanical property prediction, Marani and Nehdi [5] utilized a dataset of 154 cement-based mixtures with phase change material microcapsules and various machine learning regression algorithms to predict the compressive strength of composites, achieving superior accuracy. Sharma et al. [6-7] investigated the effect of filler aspect ratio on the fracture toughness of glass-filled epoxy composites under impact loading using ANN. They applied a multi-layer perceptron feedforward network to predict the stress intensity factor history, achieving a 91% prediction accuracy. Wang et al. [8] proposed a standard ANN model for predicting the fracture behavior of carbon fiber-reinforced polymer laminates under continuous wave laser heating and pre-tensile loads. Shabley et al. [9] explored four machine learning techniques—logistic regression, support vector machines, gradient boosting on decision trees, and gradient boosting on random forests—to predict the failure of composite materials. Yin and Liew [10] presented machine learning-assisted models for determining the interfacial properties of fiber-reinforced composites based on previous micro-bond tests. Natrayan and Kumar [11] used an integrated ANN and Taguchi approach to optimize the squeeze cast process parameters of AA6061/Al2O3/SiC/Gr hybrid composites, achieving 95% accuracy in predicting hardness and tensile strength. Several studies focused on ANN optimization and novel applications. Nikzad et al. [12] applied the Taguchi design of experiment method to optimize an ANN model for predicting the elastic properties of short fiber-reinforced composites, demonstrating the method's efficiency in resource-constrained scenarios. Al-Waily et al. [13] investigated fatigue characterization of nanoparticle-reinforced composites using ANN to validate experimental results and predict behavior under different nanoparticle percentages. Devadiga et al. [14] used ANN and microstructural evolution analysis to predict the density and hardness of multi-walled carbon nanotube composites produced by powder metallurgy, confirming the technique's accuracy. Additionally, some researchers [15–16] have provided a comprehensive review of AI applications in forecasting the mechanical properties of various types of composites. Their study explored various machine learning and deep learning techniques used for predictive modeling. This body of research highlights the growing role of artificial intelligence and ANN-based approaches in advancing composite material characterization, damage detection, and performance prediction.

Based on the literature review of the previously cited papers, no research was found that investigates the effect of graphite additives on the mechanical behavior of composites using an artificial neural network (ANN) model. Since this additive is widely applicable in many industrial applications, especially in transition composite pipes for petrochemical condensates, therefore, the primary objective of this study is to examine the impact of varying weight percentages of graphite additives on the mechanical properties of epoxy resin specimens exposed to different types of water, using an ANN framework. Traditional methods require numerous experimental tests to study the behavior of composite materials under various environmental conditions. In this study, using an ANN model significantly reduced the number of required experimental tests. To achieve this, epoxy resin specimens were prepared with different graphite weight percentages (0, 5, 10, 15, and 25 wt.%). The mechanical behavior of these specimens was evaluated by assessing their water absorption characteristics after immersion in various water types: potable water (PW), distilled water (DW), a 10 vol.% alkaline solution (NaCl), and a 10 vol.% acidic solution (HCl), following ASTM D570-98 [17]. Mechanical properties were measured through three standardized tests: Barcol hardness (BH) (ASTM D2583 [18]), impact strength (IS) (ASTM D256

[19]), and heat deflection temperature (HDT) (ASTM D648 [20]). Experimental data used as input and output for the ANN model sourced from Ref. [21]. The numerical model, developed using ANN and validated against experimental datasets, reliably predicts the mechanical behavior of epoxy resin with graphite additives when exposed to different water types. This predictive capability eliminates the need for extensive traditional experimental testing.

2. Artificial Neural Network Modelling Technique

2.1. Architecture and Algorithm

Artificial neural networks (ANNs) are a branch of artificial intelligence (AI) that automate learning by analyzing collected data [1]. ANNs typically consist of three primary layers: an input layer, one or more hidden layers, and an output layer. One of the most fundamental types of ANNs is the feedforward neural network (FNN), which is the foundation for many advanced architectures. A key characteristic is the unidirectional flow of information—from the input layer to the output layer—without any cycles or feedback loops (as shown in Fig. 1).

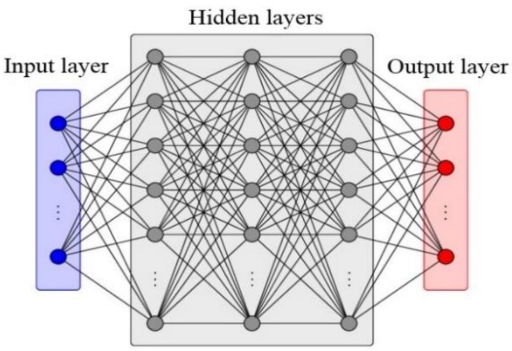

Fig. 1. A feedforward neural network schematic representation

In this research, the Backpropagation (BP) algorithm was used. A common training algorithm for ANNs is the BP algorithm, which is based on the gradient method. This approach allows the network to learn complicated, nonlinear associations between input and output. BP relies on the idea of propagating data through the network and transmitting errors backward. For each hidden layer and output layer neuron, denoting its input value as and output value as,

$$y = f\left(\sum_{i=1}^{n} \omega_i x_i - \theta\right) \tag{1}$$

In the output layer, the model processes the data received from the hidden layer and restricts the output value within the range (0,1). The hidden layer enhances the nonlinearity of the ANN model, allowing for a more accurate simulation of the correlations between the input parameters and the output value [8]. In this structure, ω_i represents the connection weight between a neuron and each neuron in the previous layer, θ is the bias of the neuron, n is the number of data points, and f denotes the transfer function, which is a sigmoid function as defined in Eq. (2).

$$f(x) = \frac{1}{1 + e^x} \tag{2}$$

The performance metric for the BP algorithm is R-squared (R2), Mean Absolute Error (MAE), Mean Squared Error (MSE), and Root Mean Square Error (RMSE), which are calculated as follows: [12,16]

$$R^2 = \left(1 - \frac{\sum_{i=1}^{n}(T_i - P_i)^2}{\sum_{i=1}^{n}(T_i - \bar{P})^2}\right) \times 100 \tag{3}$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}(T_i - P_i) \tag{4}$$

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(T_i - P_i)^2 \tag{5}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(T_i - P_i)^2}{n}} \tag{6}$$

where, T_i is the target value (measured experimental value), P_i is the predicted value and $\bar{P}$ is the mean of the response values.

In this model, we considered the weight percentage (wt.%) of graphite additive and the type of immersion water as input parameters to train and test the ANN model, with values of mechanical properties (BH, IS, and HDT) as output parameters (Table 1).

Table 1. Levels of input parameters of the numerical model

Factors	Levels				
	One	Two	Three	Four	Five
wt.% Graphite additive	0	5	10	15	25
Type of water	Dry specimen	PW	DW	Alkaline solution	Acidic solution

2.2. Neural Network Training

The experimental dataset was taken from Ref. [21] and contains 255 samples for different levels and factors used as input/output for training the ANN model. The study is divided into two significant parts. In the first section, due to the increased use of graphite as an additive in epoxy resin in various industries, especially in gas and petrochemical industries, they tested the water absorption properties of the epoxy resin containing different weights of graphite additive. They used epoxy resin with the commercial code EPIRAN-06-EPL with HA-11 hardener. The graphite powder utilized was BG706, provided by ARMINA Engineering Co. in Iran. This evaluation was conducted using the standard ASTM D570-98 method for exposure to different types of water. To achieve this, epoxy resin and hardener were mixed in a weight combination ratio of 15 units of hardener with 100 units of resin, as recommended by the supplier. The mixture was agitated for 3 minutes. Subsequently, the desired weight percentage of graphite powder was added to the resulting liquid, and the composite was molded into specimens using specialized molds with suitable geometric shapes for mechanical testing. To ensure optimal strength and curing, the specimens were cured at room temperature for 7 days, following the manufacturer's instructions. Their data showed a classical Fickian pattern of water uptake, with an R^2 value of 0.99. Additionally, in the second section of the study, the effect of water absorption on the mechanical properties of epoxy resin specimens has been investigated. Barcol hardness (BH), impact strength (IS), and heat deflection temperature (HDT) tests were conducted following the ASTM standard methods to attain this. It found that all considered mechanical properties were dependent on water uptake. From Ref. [21] for detailed information concerning the experimental procedures. See Ref. [21] for detailed information concerning the experimental procedures.

In this paper, the ANN model was developed using the 'nntool' in MATLAB R2022a. The network is designed with three hidden layers, which enhance its ability to model complex functions and capture deep, hierarchical patterns in various datasets. However, careful regularization is necessary to prevent overfitting [12, 22]. Each hidden layer was assigned 30 neurons, providing increased capacity to recognize intricate patterns in the data. While this setup is beneficial for solving complex problems, it also demands more computational resources and careful tuning to mitigate the risk of overfitting [12, 23]. Moreover, rectified linear unit (ReLU) is considered the activation function. Relu is popular due to its simplicity and effectiveness in mitigating the vanishing gradient problem. It speeds up training but can suffer from dead neurons [12, 22]. In addition, for the optimizer, Adam is used, as it combines the advantages of two other extensions of stochastic gradient descent [12, 23]. Also, the learning rate is set to 0.001, which ensures stable convergence and helps fine-tune the network. It reduces the risk of overshooting the minimum [12, 24]. Finally, the training function (trainlm) is selected. This function is a network training function that updates the weight and bias values according to Levenberg-Marquardt optimization. This training function is often the fastest backpropagation algorithm and is highly recommended as a first-choice supervised algorithm, although it does require more memory than other algorithms.

3. Results and Discussions

Before using experimental data for training the ANN model, to avoid biased responses, all inputs, including parameters of Table 1, and outputs, including values of BH, IS, and HDT, are normalized using the following equation:

$$N = \frac{X_i - \text{Minimum } of\ X}{\text{Maximum } of\ X - \text{Minimum } of\ X} \quad (7)$$

Normalization applied to the input data, where N represents the normalized value, X denotes the training data, and X_i is the value of each input data point in the training set *i= 1,2,3,….* The normalized values range between 0 and 1. To retrieve the original values, reverse normalization operations (Eq. (7)) were performed. The data points were randomly divided into three sets: 80% for training, 15% for validation, and 5% for testing. The ANN algorithms were executed on a laptop with the following specifications: 16 GB DDR4 RAM, Intel Core i5-5200U CPU, Intel(R) HD Graphics 5500 with 4 GB dedicated VRAM, running Windows 10, and equipped with a 1 TB SSD for fast data access.

Specifically, we chose to stop early with a patience = 200 criterion to reduce the risk of over-fitting the ANN algorithm. This technique is beneficial for preventing overfitting, as it allows early stopping to ensure that the neural network performs well on both training and validation data. This number of epochs is referred to as the 'patience' parameter, which specifies how many times training will continue without improvement in validation performance before stopping, preventing the model from stopping early and causing an underfit model, and preventing it from training too long and causing an overfit model. In neural network training, for example, model performance is constantly evaluated by tracking overfitting on a held-out validation set.

During training, the loss on the training set typically decreases, indicating that learning occurs. However, if the model begins to overfit the training data, its performance on the validation set may deteriorate. To address this, early stopping was implemented. If the validation loss starts increasing, it signals a decline in the model's generalization ability. A patience parameter of 200 epochs is applied, allowing the model to continue training for up to 200 additional epochs after the first increase in validation loss. If the validation loss continues to increase beyond this limit, training is halted to prevent further overfitting. This approach ensures that the model remains fair, balanced, and efficient when applied to unseen conditions, achieving optimal accuracy and performance. As previously mentioned, the trained model was evaluated based on mean absolute error (MAE), mean squared error (MSE), root mean squared error (RMSE), and the correlation factor (R). The correlation factor (R) was computed using the MATLAB software package, while MAE, MSE, and RMSE values were determined using Eqs. (4-6). The regression plots for all components of the mechanical behavior, obtained from the ANN model, are presented for the training and validation sets in Figs. 2-4.

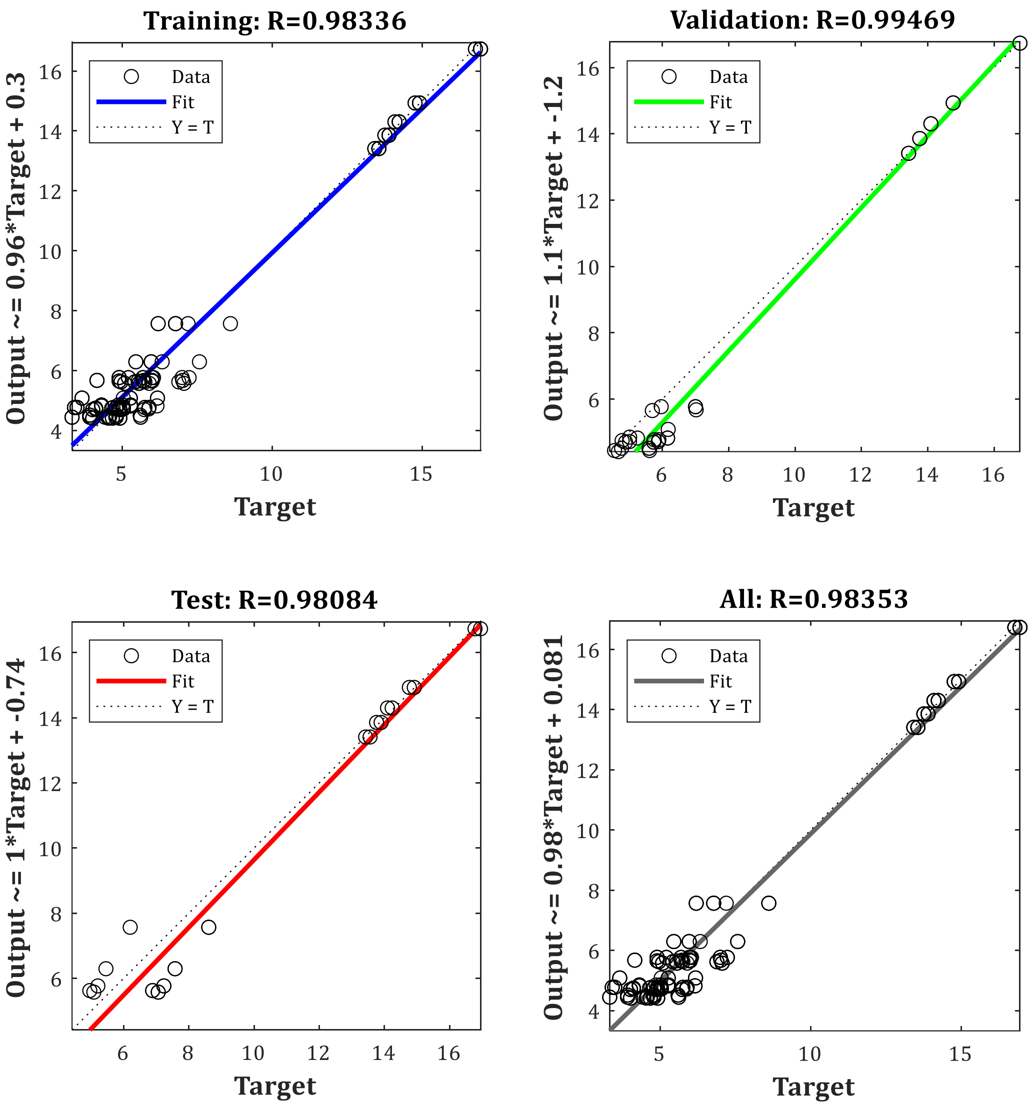

Fig. 2. Regression fit and R values for training, testing, and validation for impact strength

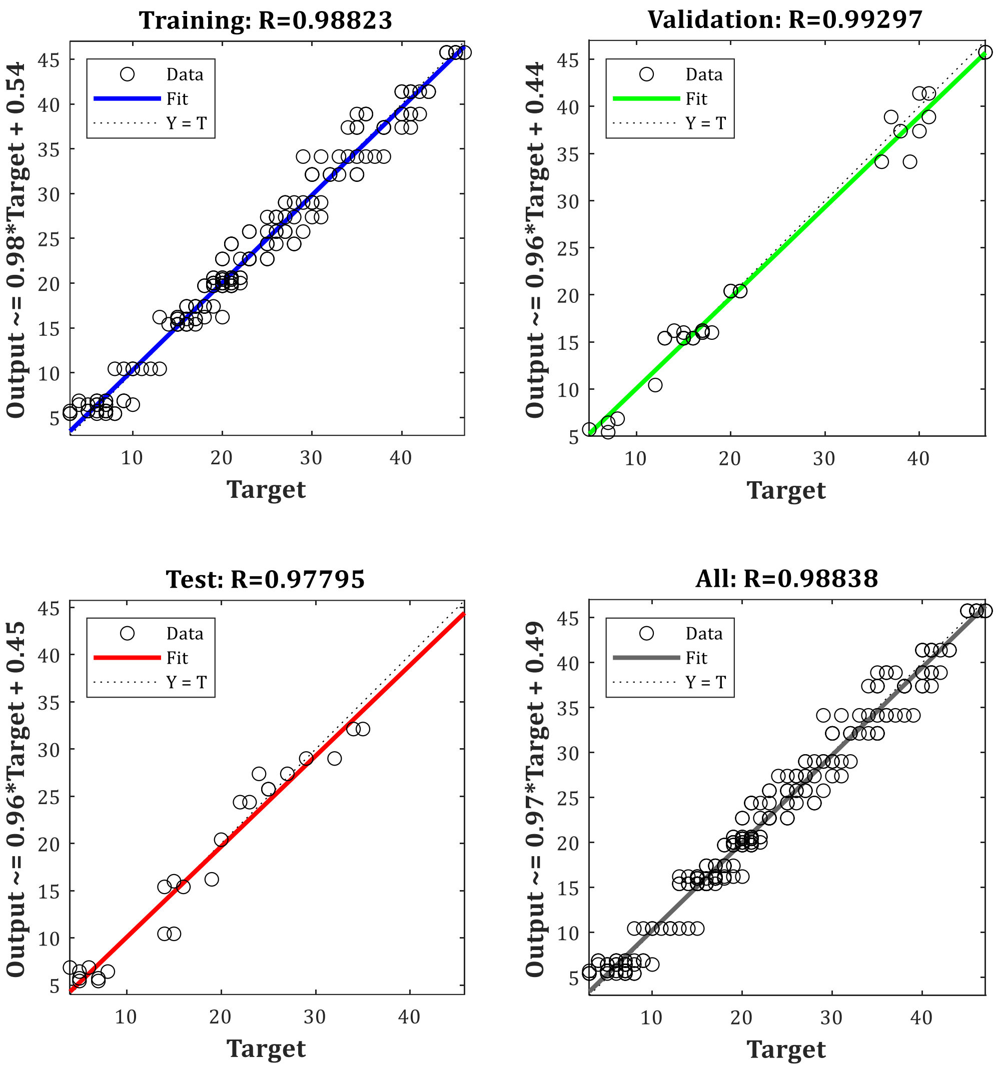

Fig. 3. Regression fit and R values for training, testing, and validation for barcole hardness

The regression plots for BH in the dataset (Fig. 3) are more dispersed than those of other mechanical behaviors. This is the case because this mechanical response, which is related to the material's surface hardness, is more variable. From a practical point of view, this means that small changes in the inputs (wt.% Graphite additive and type of water) can lead to a more significant change in this response than in the different mechanical properties. In simple terms, a higher sensitivity to the input parameters is believed to exist for this mechanical behavior than for the other mechanical properties. In other words, and loosely speaking in machine learning terms, the broader the distribution of the training data, the more difficult it is for the model to make accurate predictions, resulting in higher residuals and greater variability in the regression plots. Thus, the larger spread of BH in the regression plots is likely due to the wider distribution of this property in the training data compared to the other properties. Even though ANNs can capture nonlinearities fairly well, high variance in the output data can reduce the model's generalization capability, leading to degraded performance when the model encounters test data or out-of-sample data.

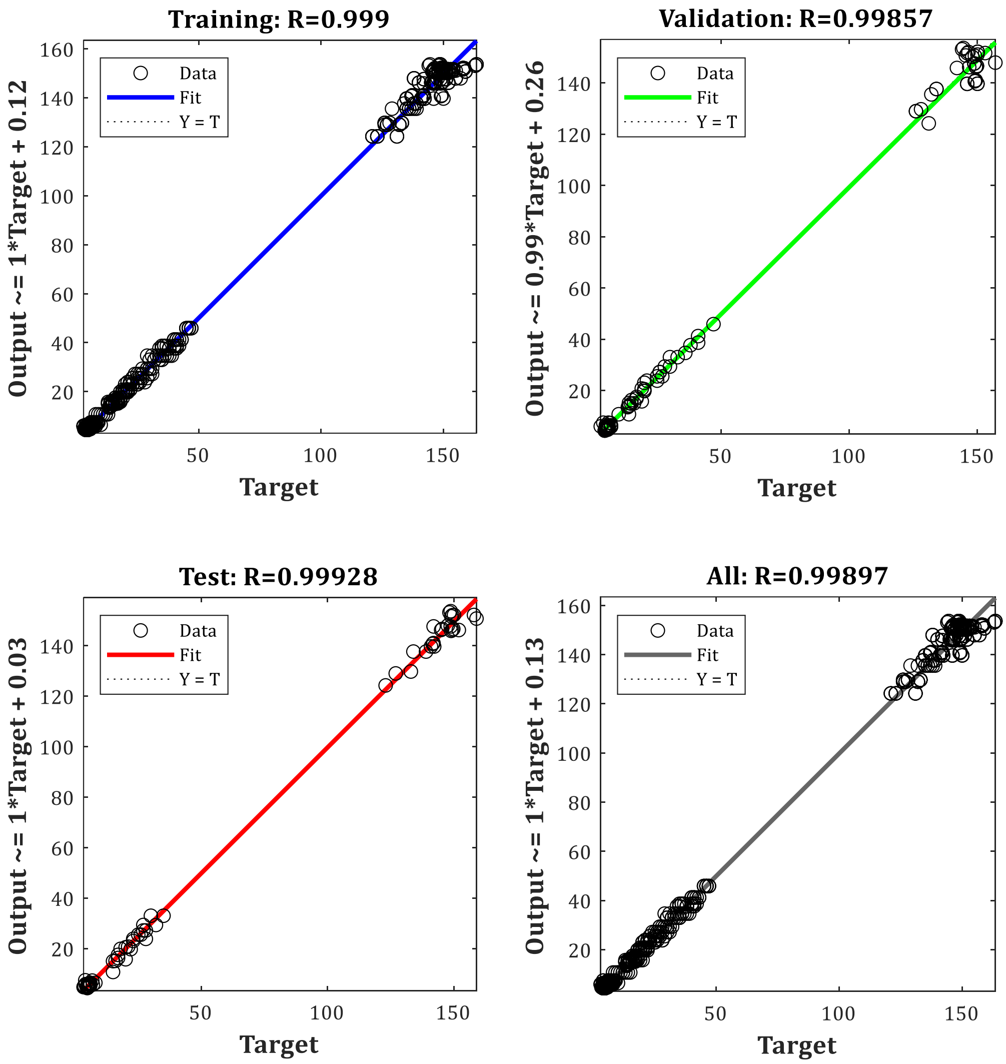

Fig. 4. Regression fit and R values for training, testing, and validation for hot deflection temperature

Table 2. Performance matrices of the proposed ANN for the simultaneous prediction of the mechanical behavior of the specimens exposed to water absorption

Component	Train				Test			
	R^2, %	MAE	MSE	RMSE	R^2, %	MAE	MSE	RMSE
Impact Strength	96.70	0.053	0.005	0.070	96.20	0.052	0.006	0.077
Barcole Hardness	97.66	0.137	0.029	0.170	95.63	0.135	0.032	0.178
Hot Deflection Temperature	99.80	0.018	0.002	0.044	99.80	0.018	0.002	0.044

Based on the evaluation data reported in Table 2 for the test set, the proposed ANN model can make reasonable predictions for unseen data points. Furthermore, the values of the evaluation factors MAE, MSE, and RMSE were deemed satisfactory, as they were close to zero. After ensuring the accuracy of the ANN model based on the evaluation parameters in Table 2, with an accuracy of over 95% for predicting the mechanical properties of epoxy resin with different weight percentages of graphite additive, the model's accuracy for each studied case determined by comparing the available experimental data with the predicted values of the ANN model for various mechanical properties. Figures 5–7 illustrate the comparison between experimental results and ANN predictions for BH, HDT, and IS, respectively, across different graphite weight percentages exposed to PW, DW, alkaline solution, acidic solution, and dry conditions.

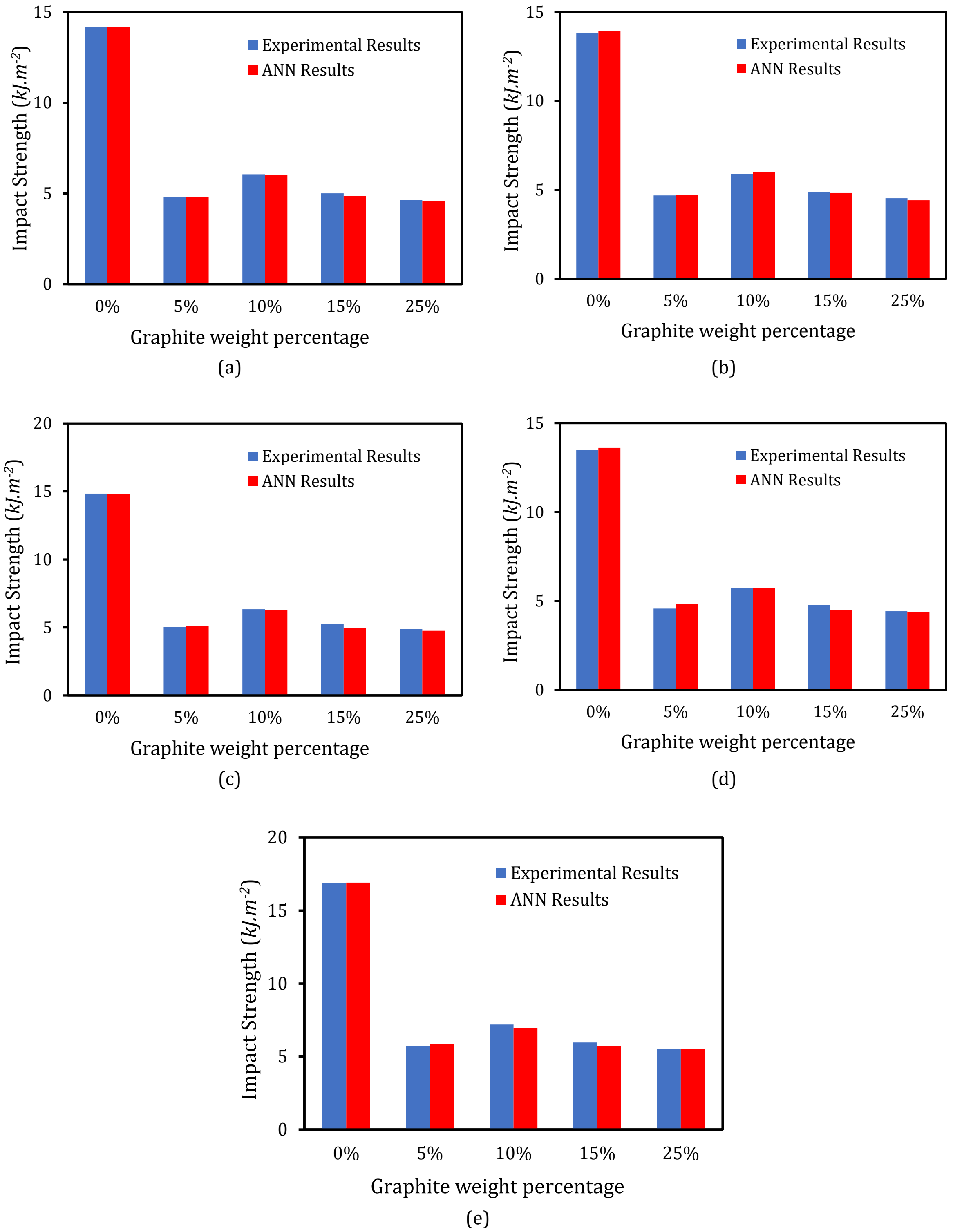

Fig. 5. Comparison between experimental and ANN impact strength results for different graphite weight percentages exposed in (a) potable water, (b) distilled water, (c) alkaline solution, (d) acidic solution, and (e) dry specimen

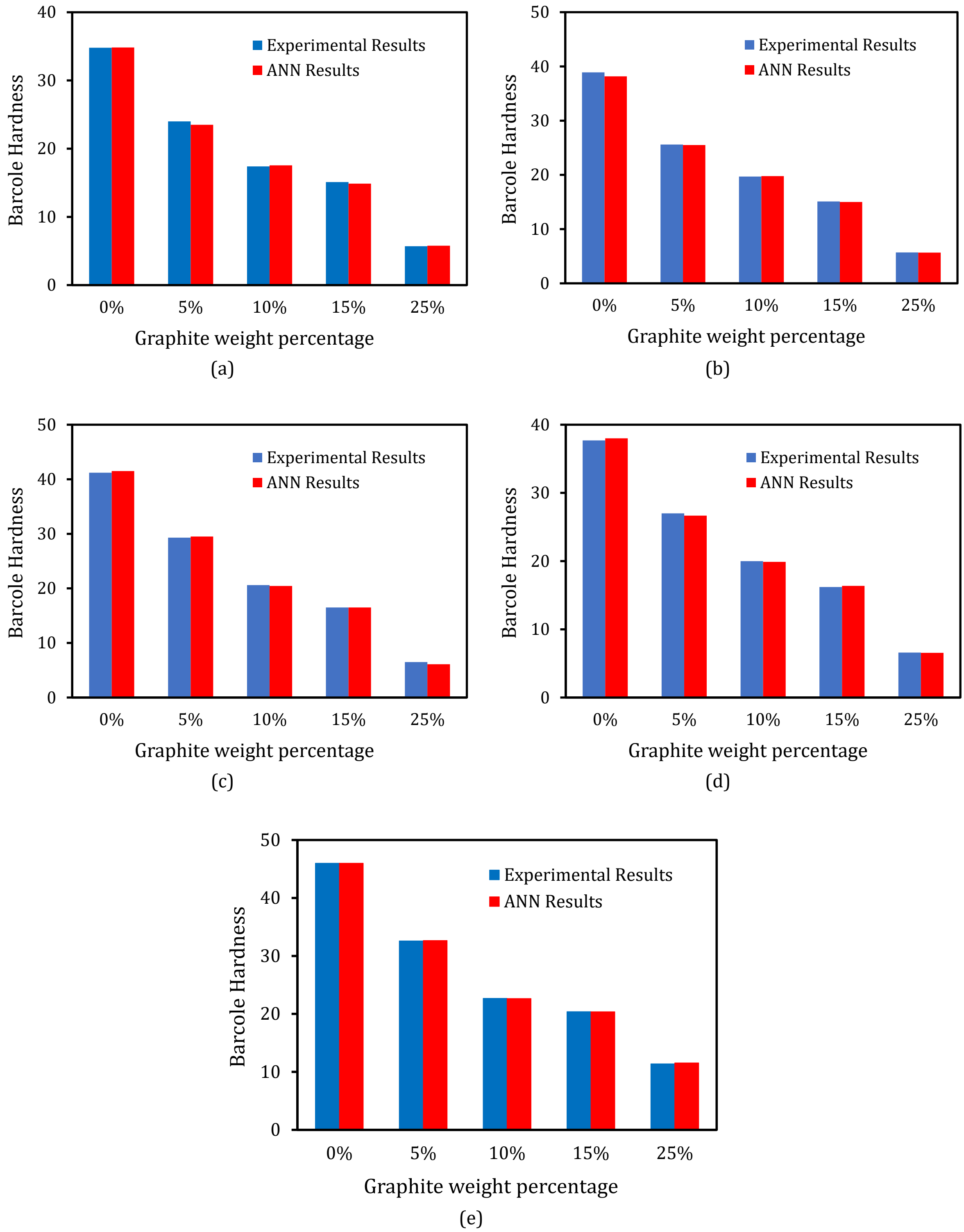

Fig. 6. Comparison between experimental and ANN barcole hardness results for different graphite weight percentages exposed in (a) potable water, (b) distilled water, (c) alkaline solution, (d) acidic solution, and (e) dry specimen

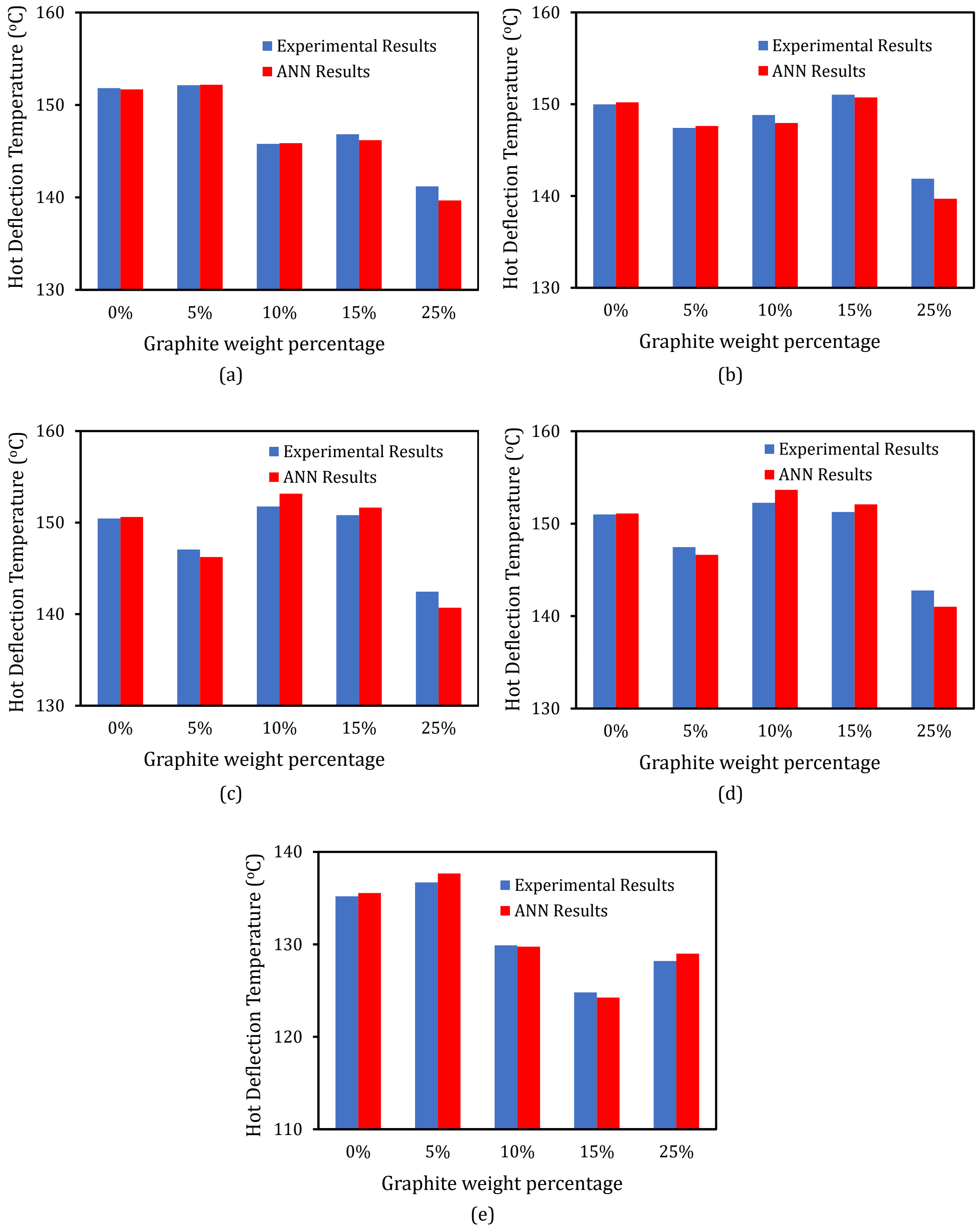

Fig. 7. Comparison between experimental and ANN hot deflection temperature results for different graphite weight percentages exposed in (a) potable water, (b) distilled water, (c) alkaline solution, (d) acidic solution, and (e) dry specimen

Since investigating the effects of graphite additives on the mechanical behavior of epoxy composites is not the main objective of this paper, only some key findings from the experimental results are summarized here; more detailed explanations are found in Ref. [21]. For all weight percentages of graphite additive, Barcol hardness decreases by approximately 16% after moisture absorption compared to the values before immersion. The smallest reduction in Barcol hardness was observed in samples immersed in alkaline water. The deflection temperature of immersed samples is higher than dry specimens, with no significant variation based on the type of water. However, under moisture conditions, the deflection temperature is lower for samples with different graphite contents compared to pure resin samples. The impact strength of immersed samples, with varying graphite weight percentages, decreases by about 16%.

According to Figs. 5-7, ANN-predicted data of three mechanical properties of epoxy resin with graphite additive were compared with experimental ones. As observed in these figures, the errors between the experimental and ANN-predicted values for Barcol hardness at 0, 5, 10, 15, and 25 wt% graphite additive are 1.88%, 2.01%, 0.89%, 1.40%, and 1.36%, respectively. Moreover, the differences between the actual and predicted values of heat deflection temperature for 0, 5, 10, 15, and 25 wt% graphite additive are 0.26%, 0.70%, 0.92%, 0.54%, and 1.23%, respectively. Finally, for impact strength at 0, 5, 10, 15, and 25 wt% graphite additive, the discrepancies between the experimental and ANN-predicted data are 0.90%, 5.70%, 3.18%, 5.10%, and 2.56%, respectively. These differences in the range of 1-5% can be attributed to experimental errors. So, these accurate predictions demonstrate the reliability of the ANN model. This will enable the use of the ANN technique to predict other wt% graphite additive levels not tested experimentally (unseen data).

The primary quality identifier of an artificial neural network is its generalization ability, its ability to use the input to accurately predict the output for data never seen in the training set, which is assessed through dataset validation. The simulation was performed to predict the values of Barcol hardness, heat deflection temperature, and impact strength before and after immersion in different types of water for 20, 35, and 45 wt.% graphite additive. Table 3 shows the ANN-predicted values of the studied mechanical properties of specimens for unseen experimental data.

Table 3. ANN predicted values of unseen data for 20, 35, and 45 wt.% graphite additive

wt.% Graphite additive	Type of water	Barcole Hardness	Hot Deflection Temperature	Impact Strength
20	Dry specimen	36.394	128.627	14.186
	Potable water	28.782	144.832	4.515
	Distilled water	21.170	142.499	5.794
	Alkaline solution	13.558	143.925	4.727
	Acidic solution	5.945	144.674	4.350
35	Dry specimen	35.780	126.710	13.934
	Potable water	28.168	142.915	4.263
	Distilled water	20.556	140.582	5.542
	Alkaline solution	12.944	142.008	4.474
	Acidic solution	5.332	142.757	4.098
45	Dry specimen	35.542	125.966	13.836
	Potable water	27.930	142.171	4.165
	Distilled water	20.318	139.838	5.444
	Alkaline solution	12.706	141.264	4.376
	Acidic solution	5.094	142.012	4.000

4. Conclusions

This study successfully demonstrated the predictive accuracy of an ANN model in estimating the mechanical properties of epoxy resin specimens with varying weight percentages of graphite additive when exposed to different water types. In the model, the weight percentage (wt.%) of graphite additive and the type of immersed water were used as input parameters to train and test the ANN, while the mechanical properties—Barcol hardness (BH), impact strength (IS), and heat deflection temperature (HDT)—served as output parameters. To evaluate the model's performance, R-squared

(R^2), Mean Absolute Error (MAE), Mean Squared Error (MSE), and Root Mean Squared Error (RMSE) are used as performance metrics. As these performance metrics were close to zero and the R-squared values were close to 1, we can be confident in the accuracy of the proposed ANN model (over 95%) for predicting the mechanical properties of epoxy resin with different weight percentages of graphite additive. The low error values and strong agreement with experimental results confirm the reliability of the proposed ANN model. These differences for Barcol hardness, heat deflection temperature, and impact strength were 1.5%, 0.91%, and 4.3%, respectively. Finally, the generalization ability of the proposed model was evaluated. We applied the ANN model to unseen data from the training set to accurately predict the output, as demonstrated by validating the dataset. It should be noted that the extrapolated predictions are intended to explore potential trends and assess the model's behavior in untested regions, rather than to claim definitive predictive accuracy in those ranges. We believe this ANN model can be effectively utilized to model improved composite materials for specialized applications, significantly reducing both computational and experimental efforts.

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Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this article. Professor Abdolhosein Fereidoon, the author of this paper, is the current Editor-in-Chief of Mechanics of Advanced Composite Structures. However, he had no role in the editorial handling or peer review process of this manuscript. The review process was independently managed by Dr. Mohammad Heidari-Rarani, an Assistant Editor of the Mechanics of Advanced Composite Structures.

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