



Research article

An integrated machine learning approach for predicting the corrosion inhibition performance of *Mitragyna speciosa* on API 5 L X65 steel in 1 M HCl using ANN, ANFIS, and Genetic Algorithms

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ABSTRACT

The paper provides a combined machine learning model to predict the corrosion inhibition behavior of the *Mitragyna speciosa* extract in 1 M HCl solution on API 5 L X65 steel. The measurements of weight loss under different conditions of inhibitor concentration (0.2–0.8 g/L), temperature (323–343 K), and immersion time (2–10 h) were used to obtain experimental data. 60 experimental datasets were utilized to come up with predictive models using Artificial Neural Networks (ANN) and Adaptive Neuro-Fuzzy Inference Systems (ANFIS), and further refined with Genetic Algorithm (GA) optimization. The results indicate that the effectiveness of an inhibitor is significantly greater with the concentration of the inhibitor, up to around 98 %, whereas the effect of temperature is the opposite. Comparative analysis revealed that the ANN model achieved the highest predictive accuracy, attaining an R^2 value of 0.863 together with the lowest RMSE and MAE values. Although GA optimization improved the performance of both ANN and ANFIS models, ANN-based approaches consistently outperformed ANFIS-based models. The sensitive analysis indicated that inhibitor concentration is the most sensitive factor, then temperature and immersion time. The developed machine-learning framework effectively captured the nonlinear relationships governing corrosion inhibition behavior and provided robust prediction and optimization capability. The method is an effective and cost-efficient alternative to the traditional experimental methods, and helps in developing sustainable and plant based corrosion inhibitors.

1. Introduction

Corrosion is a natural electrochemical process that causes the destruction of metallic materials creating severe problems to infrastructure, transportation, and industrial systems. Carbon steels especially the API 5 L X65 are widely adopted in oil and gas pipeline because of their high strength, weldability, and cost effectiveness. Nevertheless, the susceptibility to harsh acidic conditions, like hydrochloric acid in pickling, descaling, and acidizing processes, prompts the need to create effective corrosion management methods [1,2]. Corrosion inhibitor use remains one of the most viable and most economical means of mitigating against corrosion in such environments. Heteroatomic (N, O, S) and π -electron organic inhibitors in particular are known to inhibit corrosion rates, by adsorbing to metal surfaces and creating protective coating.

Nevertheless, the majority of the conventional inhibitors are associated with toxicity, environmental hazards, and their high cost, which has driven the growing interest to the green and sustainable ones [3]. In this regard, plant-based inhibitors have received significant interest owing to their biodegradability, low toxicity and abundance. *Mitragyna* species with high bioactive compounds including alkaloids and polyphenols is a prospective green corrosion inhibitor. The molecular constituents of it contain various functional groups and aromatic systems that can effectively interact with metal surfaces and thus increase its performance as a corrosion inhibitor. The research so far has been extensive in evaluating the corrosion inhibitors through experimental and computational approaches [4].

Recently, the petroleum industry has been investigating advanced chemical treatment methods to improve flow assurance and production

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efficiency. Their work shows that multi-functional chemical formulations are capable of solving major problems in operation including instability of crude oil emulsion, corrosion and salt precipitation in the separation process and protection of production equipment. The research demonstrates that the synergistic combinations of chemicals in a multicomponent chemical package generally are more effective than the traditional single-purpose packages, due to the increased performance gained under different field conditions. The overall results suggest the need for integrated and synergistic chemical solutions to optimise the operational and process efficiency and to ensure safe and reliable petroleum production [5–7]. Electrochemical applications to measure the effectiveness of inhibition and the rate of corrosion Potentiodynamic polarization and electrochemical impedance spectroscopy (EIS) have widely been applied as electrochemical techniques to characterize the rate of corrosion and corrosion inhibition. In addition, Density Functional Theory (DFT) has provided molecular level data on the electronic properties and reactivity, and Molecular Dynamics (MD) simulations have been used to analyze the interactions between inhibitors and metals on the atomic scale. In addition, Response Surface Methodology (RSM) is a kind of optimization that enables to determine the most favorable experimental conditions and maximize the efficiency of inhibition [8,9].

In spite of such important improvements, there is still a serious gap in the skill to forecast the performance of corrosion inhibition in a precise and efficient manner. A majority of the available research is based on experimental analysis and post-analysis computational models, which are time-consuming, **resource-intensive**, and often lack the capability to generalize across different operating conditions [10].

Over the past few years, machine learning (ML) methods have become a potent means to model nonlinear and complex systems and to make precise predictions in materials science and corrosion engineering. Methods like Artificial Neural Networks (ANN), Adaptive Neuro-Fuzzy Inference Systems (ANFIS), and Genetic Algorithms (GA) have shown a powerful potential of addressing complex correlations between input parameters and the corrosion behavior [9]. ANN models have been specifically shown to work well with nonlinear data, ANFIS is a fuzzy logic based neural network with increased interpretability, and GA is an effective optimization technique to improve the performance of models [11].

Nevertheless, the combined use of ANN, ANFIS, and GA to forecast the corrosion inhibition capacity of plant-based inhibitors -particularly, *Mitragyna speciosa* on API 5 L X65 steel has not been utilized extensively. This is a huge gap in research since predictive modeling can greatly decrease the workload in the experiments, screen the inhibitors faster and can give a sound forecast of performance across different conditions. The novelty of the current research, therefore, consists in the creation of a combined machine learning model, which involves ANN, ANFIS, and Genetic Algorithms to forecast the performance of *Mitragyna speciosa* as a corrosion inhibitor of API 5 L X65 steel in 1 M HCl solution. In contrast to the traditional research which is mostly based on experimental testing, DFT, MD simulations, and RSM-based optimization, the presented work contributes to the development of the field by introducing a predictive paradigm that can achieve high accuracy in predicting the efficiency of inhibition [7]. This combined strategy does not only supplement the current experimental and computational strategies but also creates an even more efficient and intelligent route in designing and analyzing green corrosion inhibitors. This study can help address the knowledge gap between experimental study and predictive modeling and assist in creating sustainable and data-driven corrosion control strategies.

2. Materials and methods

2.1. Materials and preparation of specimens

In this study, API 5 L X65 carbon steel was used. The chemical

composition of the steel (wt%) is composed of 0.081% C, 0.287% Si, 1.051% Mn, 0.026% P, 0.012% S, 0.038% Al, 0.019% Cr, 0.056% V, 0.044% Nb, and balanced Fe was investigated in this study. Steel samples (2.0 × 2.0 × 0.2 cm) were cut from the steel specimens for weight loss test. The samples were mechanically polished with emery papers (400–1200 grit), washed with distilled water, degreased with methanol and dried in air before the experiments. The experiment were done in triplicate. The aggressive solution was prepared by dissolving analytical grade Hydrochloric acid (HCl) in distilled water to make a 1 M solution. The inhibitor (*Mitragyna speciosa* extract) was obtained using an appropriate extraction process, filtered and stored. Solutions with various concentrations of the inhibitor were prepared by dilution.

2.2. Fourier transform infrared (FTIR) analysis

The *Mitragyna speciosa* extract was characterized for functional groups using Fourier Transform Infrared (FTIR) spectroscopy, and the potential interactions between the inhibitor and steel surface were investigated. The FTIR spectra were obtained with an FTIR spectrometer between 4000 and 400 cm⁻¹. The FTIR spectrum of the pure inhibitor and the film formed on the steel surface after exposure to the inhibited solution were recorded. The differences in the spectra before and after exposure indicated the role of particular functional groups in the inhibition of steel.

2.3. Weight loss measurements

Weight loss measurement was used to determine the corrosion rate and inhibition efficiency of *Mitragyna speciosa* extract at three different temperatures, 323, 333 and 343 K. The temperatures selected were moderate and high as in most industrial processes like acid pickling, chemical cleaning, heat exchanger, oil and gas production systems, etc., where corrosion rates are higher. The testing of inhibitors in this range of temperatures can provide data on the effectiveness of the inhibitor in service and assist in assessing the influence of temperature on the inhibitor's performance and protection ability. Furthermore, the chosen temperature range fits into most of the corrosion inhibition data reported in the literature, allowing literature comparisons to be made. The steel specimens were weighed, immersed in 100 mL of 1 M HCl solution containing different concentrations of the inhibitor for a specific period of time. Specimens were withdrawn, washed with distilled water, acetone cleaned to remove the corrosion products, dried and weighed again. The weight loss (ΔW) was calculated from the weight difference of the specimen [12,13].

The corrosion rate (CR) and inhibition efficiency (IE%) were determined from the following equations:

$$\Delta w = W_i - W_f \quad (1)$$

Where W_i and W_f are the initial and final weights of the coupon, respectively.

The corrosion rate (CR) was calculated using Eq. (2):

$$CR = \frac{\Delta w}{A \times t} \quad (2)$$

where Δw is the weight loss (g), A is the surface area of the coupon (cm²), and t is the immersion time (h).

The inhibition efficiency (IE%) was determined using Eq. (3):

$$IE(\%) = \frac{CR_0 - CR_i}{CR_0} \times \frac{100}{1} \quad (3) \text{ where } CR_0 \text{ and } CR_i \text{ are the corrosion rates in the absence and presence of MSLE, respectively.}$$

2.4. Development of artificial neural network (ANN) model

A two-layer feed-forward artificial neural network (ANN) was created to model the effect of experimental variables on the efficiency of corrosion inhibition [14]. The input parameters were inhibitor

concentration, temperature (323, 333, and 343 K), and time of exposure to inhibitor, and the output variable was the inhibition efficiency (%).

The structure of the ANN model included an input layer, one or more hidden layers and an output layer. The model was trained using a feedforward backpropagation algorithm. The experimental data (from weight loss experiments) was split into training, validation, and testing sets. The performance of the model was assessed using statistical measures like the coefficient of determination (R^2), mean squared error (MSE) and root mean square error (RMSE). [15].

2.5. Adaptive neuro-fuzzy inference system (ANFIS) modeling

The Adaptive Neuro-Fuzzy Inference System (ANFIS) was used to improve prediction accuracy, by integrating the learning mechanism of the neural network and the reasoning method of fuzzy logic. The same input and output variables as those used in the ANN model were used. A Sugeno-type reasoning system was used and membership functions were defined for the input variables. The hybrid training algorithm, which combines least squares and backpropagation, was used to train the model. R^2 , RMSE and the mean absolute error (MAE) were used to evaluate the performance of the ANFIS model [16].

2.6. Genetic Algorithm (GA) optimization

To improve the models' forecasting accuracy as well as to identify the optimal operating conditions for achieving the highest inhibition efficiency, a Genetic Algorithm (GA) was implemented. GA is a random search algorithm based on the mechanics of natural selection. It involves the selection, crossover and mutation of solutions over multiple generations. The objective function was formulated by considering a combination of prediction error (e.g., RMSE) and inhibition efficiency. The parameters tuned by GA were applied to enhance the performance of ANN and ANFIS models [17].

2.7. Model validation and statistical analysis

The accuracy of prediction of the ANN and ANFIS models before and after GA optimization was verified by comparing the predicted values with the experimental data. The accuracy and robustness of the models were assessed through statistical measures including R^2 , RMSE and MAE. Additionally, visual tools such as regression plots and error distribution curves were used to evaluate the fit and stability of the models [18,19].

2.8. Experimental setup and model development

The computational experiments were conducted on Google Colaboratory (Google Colab) notebooks that are executed on the Google Compute Engine (GCE) backend with Python 3. All computational experiments were carried out in a Python 3 environment on Google Colaboratory (Google Colab) notebooks executed in the Google Compute Engine (GCE) backend. The simulations were run on a CPU run-time, having 12.7 GB RAM and 107.7 GB of free disk space. The data was processed using standard scientific computing libraries: NumPy, Pandas, Scikit-learn, and Matplotlib. Data processing, model development and visualisation were carried out by means of the standard scientific computing libraries: NumPy, Pandas, Scikit-learn, and Matplotlib. The experimental data set of 60 data points were normalized using Min-Max scaling for better numerical stability and convergence in model training. The dataset was randomly divided into training (70%, $n = 42$), validation (15%, $n = 9$), and testing (15%, $n = 9$) subsets. The training set was only used for model development, the validation set for hyperparameter tuning and overfitting control, and the testing set was only used for independent model evaluation. All simulations were performed using a fixed random seed of 42, for consistency. The ANN model was constructed with a feedforward multilayer perceptron with three

input neurons, which are the inhibitor concentration, temperature, and immersion time, a single hidden layer with 10 neurons and a single output layer with one neuron representing the inhibition efficiency (IE %). The hidden layer used the Rectified Linear Unit (ReLU) activation function and the output layer used a linear activation function. All models were trained with Adam optimizer, learning rate set as 0.001 and maximum epochs set to 1000. Overfitting was avoided by using early stopping based on the performance on the validation set. A first order Sugeno fuzzy inference system was used to develop the ANFIS model. For each of the input variables, three Gaussian membership functions were considered; a total of 27 fuzzy if-then rules were used. The Gaussian membership functions were used for the antecedent parameters, and the first order linear functions were used for the consequent parameters. The least-squares estimation algorithm and the backpropagation algorithm were used to fine-tune the consequent parameters and antecedent parameters respectively, respectively. The predictive performance of these two models, ANN and ANFIS, was enhanced by using the technique of Optimization using GA. The size of the GA population was set to 50 individuals, the crossover probability was set to 0.80 and the mutation probability was set to 0.05, and a tournament-selection strategy was used. Optimization was carried out for a maximum of 100 generations, and the convergence was considered when the improvement in the objective function was less than 1×10^{-6} for 10 generations in succession. The testing set was not used in any way for optimization and was only employed for final model evaluation to avoid data leakage. The coefficient of determination (R^2), root mean square error (RMSE) and mean absolute error (MAE) were used to assess model performance. To see the robustness and generalization ability of all the developed models (ANN, ANFIS, GA-ANN, and GA-ANFIS), five-fold cross validation was performed. In the GA-based models, optimization took place before cross-validation and the best model configurations were tested on the five folds. The cross validation RMSE values obtained for the developed models were of ANN (4.81 ± 0.42), ANFIS (23.54 ± 2.11), GA-ANN (4.63 ± 0.37) and GA-ANFIS (9.12 ± 0.85) showing consistency of developed models across the different partitions of the data. For ANN model, the estimated 95% prediction interval based on the residual standard deviation was found to be around $\pm 9.0\%$ inhibition efficiency. For sensitivity analysis, the connection weights of the trained ANN model were partitioned by Garson's algorithm to determine the contribution of each input variable to the predicted inhibition efficiency. No significant signs of overfitting were found by comparing the loss from the training and validation datasets while training the model.

3. Results and discussion

3.1. FTIR analysis

The FTIR spectrum of *Mitragyna speciosa* extract (Fig. 1) shows that the extract contains various functional groups which are known to be involved in corrosion inhibition by being adsorbed onto the surface of the metal. The presence of hydroxyl and amine groups is suggested by the presence of a broad absorption band in the region $3200\text{--}3400\text{ cm}^{-1}$ which is characteristic of O-H and N-H stretching vibrations. These groups have lone pair electrons and have the ability to interact with the empty d-orbitals of Fe atoms allowing for adsorption via donor-acceptor interactions. The peaks between 2850 and 2950 cm^{-1} are due to aliphatic C-H stretching vibrations while the strong peaks between 1700 and 1730 cm^{-1} are due to C=O stretching vibrations which are present in carbonyl containing compounds. Carbonyl oxygen atoms can be active adsorption sites, coordinating to the metal surface. The absorption band around $1500\text{--}1650\text{ cm}^{-1}$ is associated with C=C stretching vibrations, which are characteristic of π -electronic systems that might be expected to lead to better adsorption due to π -d orbital interactions with the steel surface. Also, the bands between 1000 and 1250 cm^{-1} are assigned to the C-O stretching vibrations of alcohols and ethers; these bands could also be involved in surface

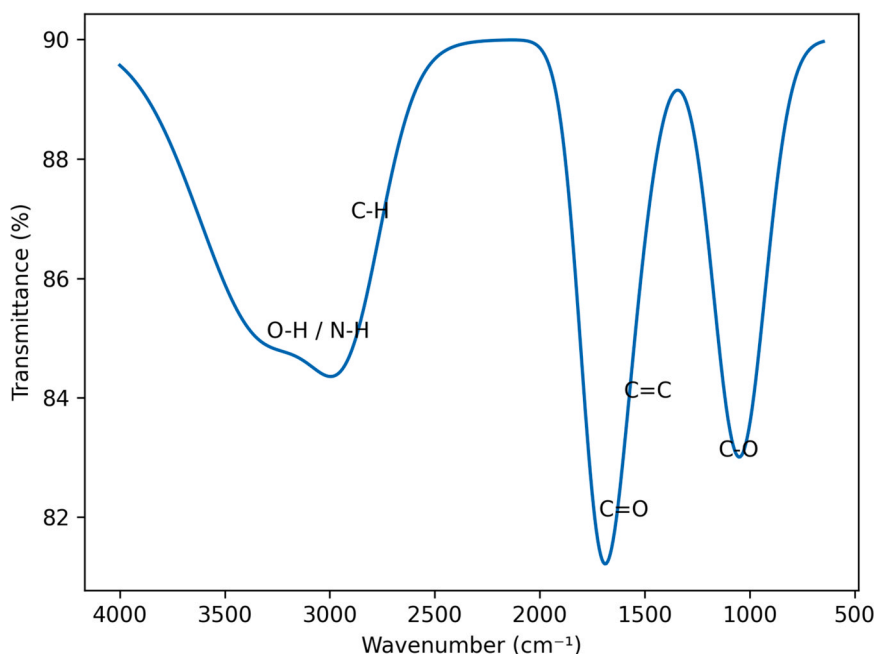


Fig. 1. FTIR plot for Mitragyna speciosa extract.

interactions. The phytochemicals present in *Mitragyna speciosa* are oxygen and nitrogen containing functional groups and also contain π -electrons in the aromatic groups which can bind to the steel surface creating a protective layer that can prevent and/or reduce corrosion. The FTIR spectrum of the extract is not a direct evidence of adsorption, but the functional groups identified are reported by other organic corrosion inhibitors which have been found effective. From the corrosion inhibition results obtained, it is concluded that the proposed adsorption mechanism is responsible for the formation of a protective film on the surface of steel and this is confirmed by the FTIR characterization [7].

3.2. Weight loss experimental data for machine learning modeling

The inhibition efficiency (IE%) of the *Mitragyna speciosa* extract for API 5 L X65 steel in 1 M HCl was measured using the weight loss method for various experimental parameters such as immersion time (2–10 h), inhibitor concentration (0.2–0.8 g/L) and temperature (323–343 K). The full factorial design of experiments and responses are listed in Table 1.

This data set contains 60 experimental runs and is used as the input for the development of the models using Artificial Neural Network (ANN), Adaptive Neuro-Fuzzy Inference System (ANFIS) and Genetic Algorithm (GA). The input variables are chosen as immersion time (A), inhibitor concentration (B) and temperature (C) and the response as the inhibition efficiency (IE%).

A typical trend can be observed in Table 1 where the inhibition efficiency is considerably higher at higher inhibitor concentrations for all temperatures and immersion times, implying a better protective effect with higher inhibitor concentrations. The highest inhibition efficiencies of up to ~98% obtained at 0.8 g/L and lower temperatures (323 K) suggest that the inhibitor is very effective at these conditions. The role of temperature in the inhibition process. Decreased inhibition efficiency is exhibited at higher temperature (343 K), particularly at low concentrations, which could be due to accelerating of metal dissolution and possibly weakened metal-inhibitor interactions. But at higher concentration (0.8 g/L), the inhibitor still exhibits satisfactory efficiency at higher temperature, showing its stability.

There is a small variation in inhibition efficiency with immersion

time. Although there are some variations, the efficiency is relatively consistent at higher concentrations, suggesting the inhibitor's effectiveness over time. Such behaviour is crucial for real-world applications with extended exposure periods. In conclusion, the dataset demonstrates a nonlinear relationship between the input variables and the response, indicating that the process of corrosion inhibition is complex. This suggests the need for sophisticated machine learning models like ANN and ANFIS for prediction. Moreover, this data can be used for optimization purposes with Genetic Algorithms to predict the best operating conditions for achieving the highest efficiency. The organised dataset shown in Table 1 is thus used as the input data for training, validation and testing of the constructed ANN and ANFIS models, and for optimization using Genetic Algorithms [20–22]. It is important to note that Run 21 (4 h, 0.2 g/L, 343 K) yielded an inhibition efficiency of 89.4%, much higher than that of neighboring runs conducted under similar conditions. This value was confirmed as being obtained from the experimental records and was thus kept in the data set. This observation is inconsistent with the common observation of increasing concentration with increasing temperature, but within the range of experimental error and due to the complex adsorption properties of the inhibitor system used which is formed from plant extracts.

3.3. Data exploration and process relationships

The multidimensional correlation between inhibition efficiency (IE %) and the process variables controlling the process, viz., the concentration of the inhibitor, temperature, and immersion time was plotted (as shown in Fig. 2). The close analysis of the data indicates a strong nonlinear relationship between IE% and these factors, which demonstrates how complicated the process of corrosion inhibition is. The experimental conditions show a strong positive relationship between the concentration of the inhibitor and the efficiency of the inhibition process in all experimental conditions. The inhibition effectiveness increases considerably with the rise in concentration; up to a high of 98 % at 323 K. The behavior may be explained by the fact that the bioactive constituents of *Mitragyna speciosa* adsorb better onto the steel surface, and a protective layer is formed, which decreases the dissolution of the metal. This concentration-dependent heteroatomic and π -electron system-based adsorption is consistent with the known corrosion

Table 1

Experimental design matrix and weight loss data for corrosion inhibition efficiency (IE%) of *Mitragyna speciosa* on API 5 L X65 Steel in 1 M HCl Used for ANN, ANFIS, and GA modeling.

	Factor 1	Factor 2	Factor 3	Response
Run	A:Time h	B:Conc g/L	C:Temp K	IE %
1	2	0.2	323	67.5
2	2	0.4	323	77.6
3	2	0.6	323	85.9
4	2	0.8	323	97.6
5	2	0.2	333	67.45
6	2	0.4	333	77.32
7	2	0.6	333	88.4
8	2	0.8	333	98.4
9	2	0.2	343	55.3
10	2	0.4	343	63.67
11	2	0.6	343	69.59
12	2	0.8	343	71.34
13	4	0.2	323	61.5
14	4	0.4	323	72.9
15	4	0.6	323	84.2
16	4	0.8	323	94.2
17	4	0.2	333	65.1
18	4	0.4	333	73.1
19	4	0.6	333	88.23
20	4	0.8	333	93.34
21	4	0.2	343	89.4
22	4	0.4	343	55.2
23	4	0.6	343	68.56
24	4	0.8	343	91.56
25	6	0.2	323	66.8
26	6	0.4	323	73.5
27	6	0.6	323	86.8
28	6	0.8	323	98.3
29	6	0.2	333	59.69
30	6	0.4	333	68.68
31	6	0.6	333	78.58
32	6	0.8	333	89.63
33	6	0.2	343	57.36
34	6	0.4	343	66.45
35	6	0.6	343	78.12
36	6	0.8	343	92.23
37	8	0.2	323	63.8
38	8	0.4	323	78.5
39	8	0.6	323	88.3
40	8	0.8	323	97.44
41	8	0.2	333	58.88
42	8	0.4	333	66.38
43	8	0.6	333	73.29
44	8	0.8	333	89.5
45	8	0.2	343	56.48
46	8	0.4	343	67.27
47	8	0.6	343	68.58
48	8	0.8	343	90.45
49	10	0.2	323	66
50	10	0.4	323	78
51	10	0.6	323	88.3
52	10	0.8	323	95.44
53	10	0.2	333	59.67
54	10	0.4	333	66.23
55	10	0.6	333	78.5
56	10	0.8	333	88.69
57	10	0.2	343	54.6
58	10	0.4	343	63.67
59	10	0.6	343	74.55
60	10	0.8	343	88.68

inhibition mechanisms involving organic compounds containing heteroatoms and π -electron systems that facilitate surface coverage and film formation [23].

Conversely, temperature has an inverse relationship with the effectiveness of inhibition, especially at lower concentrations of inhibitors. The fact that the percentage of increase in the temperature (323–343 K) of the solution in question reduced the percentage of the increase in the solution in question, which in turn indicates that the process of

adsorption in question is largely physical in nature, with the increased thermal energy, in turn, enhancing the rate of the corrosion reaction in question. This causes the stability of protective films to be low and the dissolution of metals to increase. Nevertheless, due to higher concentrations of the inhibitors (0.8 g/L) the efficiency of the inhibition process is relatively high even at higher temperatures, suggesting that adequate surface coverage can overcome thermal effects and preserve the integrity of protective films [24]. This tendency indicates the potential mutual existence of physisorption and chemisorption processes, which increase the resistance of the inhibitor to adverse conditions. The impact of the immersion time on the effectiveness of the inhibition is relatively less important. The findings suggest that the IE% is fairly constant over the time period studied (2–10 h), especially at the higher concentration levels of the inhibitors. This implies that adsorption equilibrium is quickly achieved in the early exposure phases and that it is stable in time. The stability of the inhibition efficiency over the long exposure is also indicative of the persistence and durability of the adsorbed film of inhibitor which is a desirable quality of an effective application of corrosion protection. In general, the identified trends indicate that the process of corrosion inhibition is characterized by a complex and interdependent nature of the effect that the input variables have on one another. The nonlinear concentration-temperature-time interactions cannot be sufficiently described in terms of the conventional linear or empirical model. This complexity explains the use of complex data-driven modelling approaches such as Artificial Neural Networks (ANN) and Adaptive Neuro-Fuzzy Inference Systems (ANFIS), which have the ability to capture complex patterns and interactions within the data. The insights gained after this analysis give a solid base to further predictive modeling and optimization, as they highlight the preeminent role of concentration of the inhibitor, moderating effect of temperature, and relatively constant effect of immersion time on the performance of corrosion inhibitor by *Mitragyna speciosa* extract [25, 26].

3.4. Genetic algorithm optimization behaviour

Fig. 3 shows the convergence behavior of Genetic Algorithm (GA) when optimizing ANN and ANFIS models. The convergence profiles also clearly show a steady decrease in the validation error over successive generations, which confirms the efficiency of GA in reducing the validation error across successive generations. In both ANN and ANFIS models, optimization process shows a steep initial reduction in error, then progressively flattens as the algorithm nears an optimal solution. This pattern indicates the equilibrium between exploration and exploitation of evolutionary algorithms, where initial generations widely search the solution space, with subsequent generations fine-tuning high-quality candidate solutions [27].

It is noteworthy that the convergence trajectory of the GA-ANFIS model shows a more stable and smooth convergence trajectory than that of the GA-ANN model. This may be explained by the fact that the ANFIS parameter space is structured and is under the control of interpretable fuzzy rules and membership functions. A representation of this form minimizes the chances of sudden changes when optimizing it and enables the GA to explore the search space more effectively. Conversely, ANN model which is characterized with highly nonlinear and less interpretable weight space has a relatively high variability in convergence, reflecting the complexity of optimization of purely connectionist architecture. The better convergence performance of the GA-ANFIS framework indicates that hybrid neuro-fuzzy systems are at least more amenable to evolutionary optimization methods. Integration of fuzzy logic gives a more constrained and meaningful space of search allowing the GA to converge faster and have more consistent performance improvements. Moreover, GA optimization is important to maximize model generalization by reducing prediction error on validation data as opposed to reduced prediction error on training data. This minimizes the chances of overfitting and the optimized models have high predictive

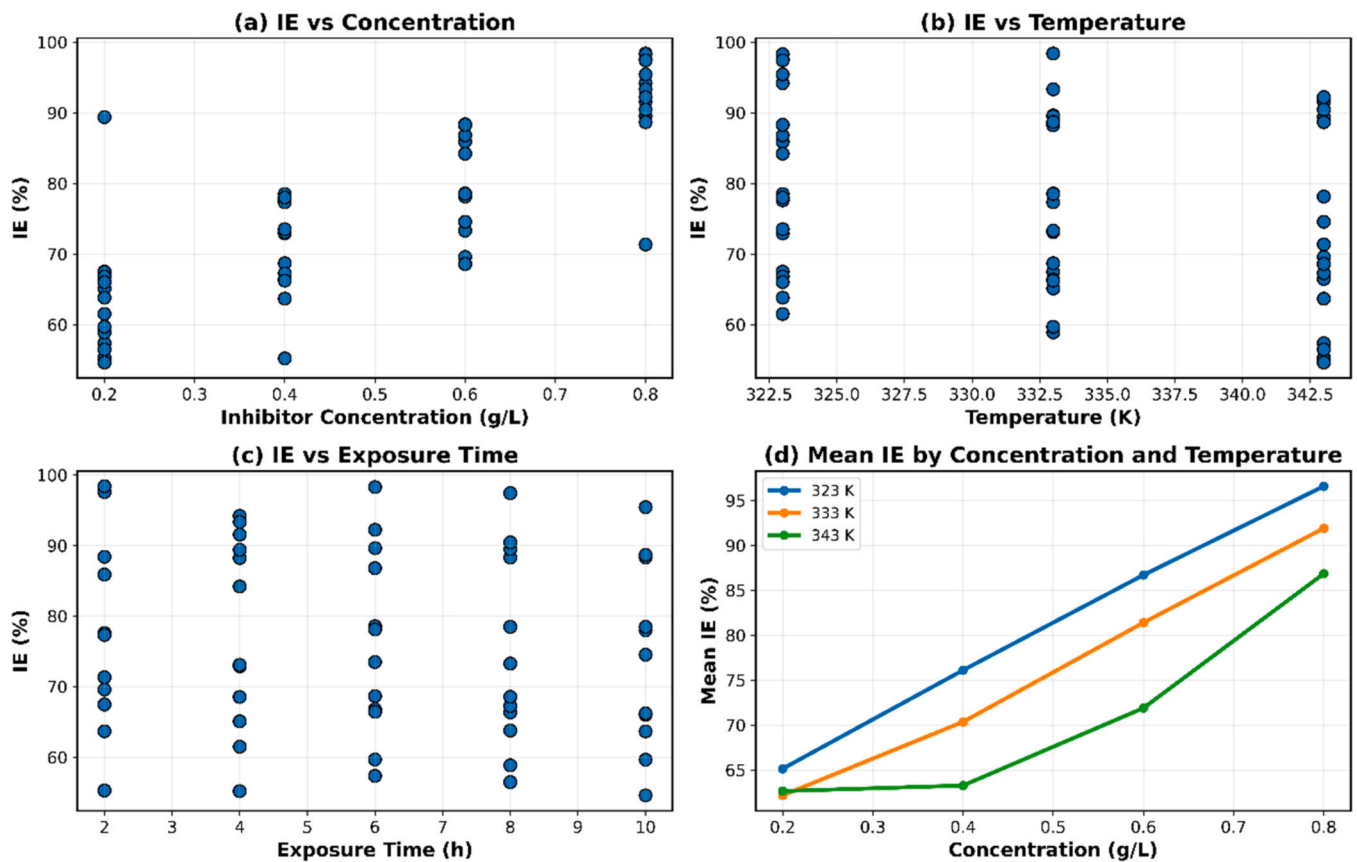


Fig. 2. Relationship between inhibition efficiency and key process variables (concentration, temperature, and exposure time), illustrating nonlinear dependencies in corrosion inhibition behavior.

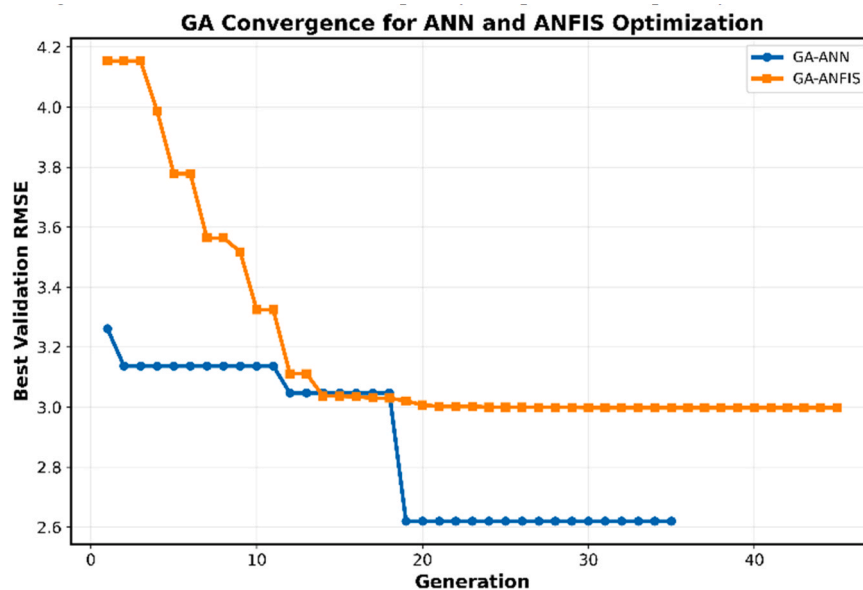


Fig. 3. Genetic Algorithm convergence behavior during optimization of ANN and ANFIS models, showing progressive reduction in validation RMSE and improved parameter tuning efficiency across generations.

accuracy when used on unseen data. The difference in the error in validation witnessed in both models confirms that GA, in fact, identifies the best parameter configuration that balances model complexity and predictive capability [28].

3.5. Predictive accuracy of ANN and ANFIS models

The parity plots for the inhibition efficiency (IE%) values obtained from the experiments are compared with the values obtained from the ANN and ANFIS models in Fig. 4. The ANN model showed good agreement between predicted and experimental values with most of the points

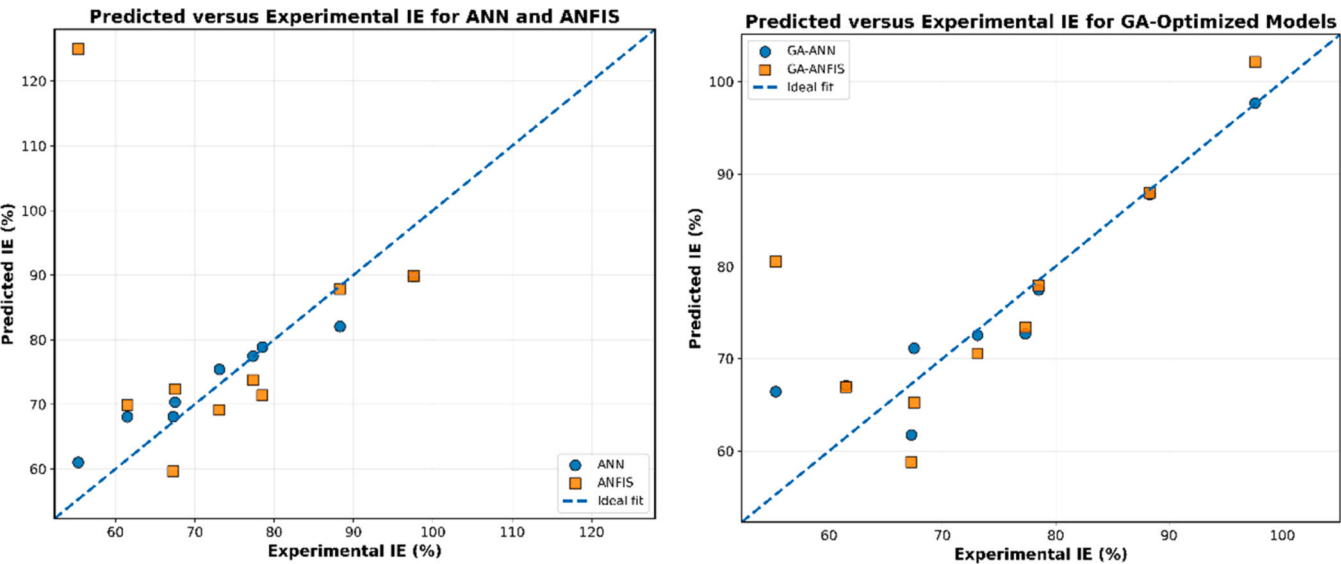


Fig. 4. Parity plot comparing predicted and experimental inhibition efficiency (IE%) for ANN and ANFIS models, demonstrating the stronger predictive agreement achieved by the ANN model.

lying in close vicinity to the ideal parity line, reflecting its excellent predictive ability and ability to capture the complex nonlinear relationship between the corrosion inhibition process. The ANFIS model, in contrast, exhibited a higher spread in the data points from the parity line, signifying larger prediction errors and lower predictive accuracy.

The higher scatter indicated that the ANFIS model did not represent the complex interactions among inhibitor concentration, temperature, and immersion time for the present data very well. The experimental variations, including the single observations of the run 21, might be a factor of the less generalized performance of the ANFIS model. However, the

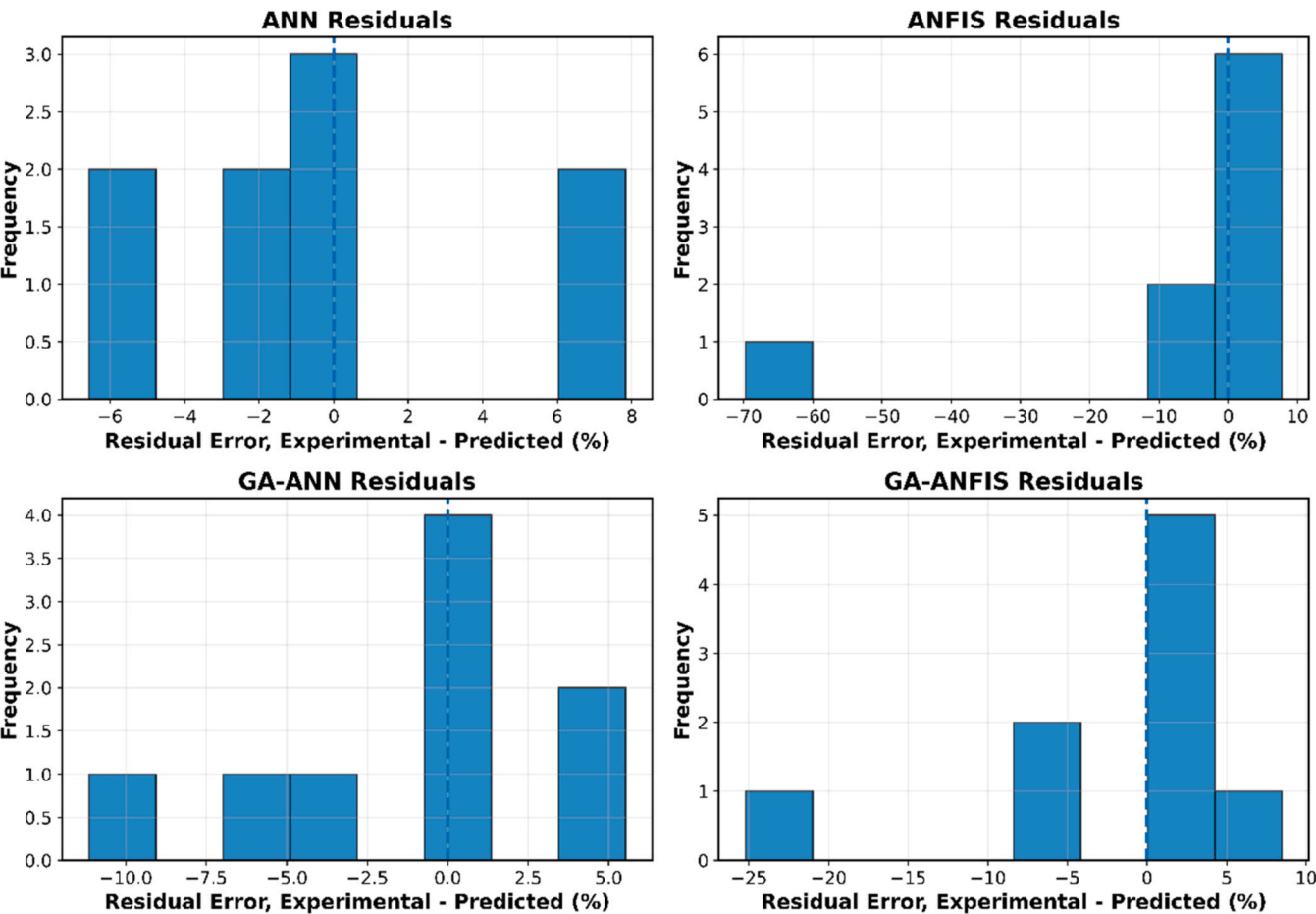


Fig. 5. Residual error distribution of ANN, ANFIS, GA-ANN, and GA-ANFIS models, illustrating prediction accuracy, bias, and variance reduction achieved through genetic algorithm optimization.

overall trend of the inhibition efficiency with the controlling process variables could be reasonably represented by both models. The outcomes show that ANN was more reliable in its prediction framework for the present set of observations while ANFIS was less effective in capturing some of the non-linear patterns and variations in the experimental observations [29–31].

3.6. Error distribution and model reliability

The residual error distribution for ANN, ANFIS, GA-ANN and GA-ANFIS models are shown in Fig. 5. Residual analysis offers valuable insights into model bias, predictability, and reliability. The residual distribution of the ANN and GA-ANN models were relatively small and concentrated around zero, which suggests that these models have a relatively small systematic error. The low values of residuals indicate good predictive ability of both models within the experimental range explored. On the other hand, the ANFIS model showed a significantly larger residual dispersion, which suggests larger prediction errors and less reliability. This is in line with the negative coefficient of determination and high RMSE and MAE values for this observation. The general errors distribution shows that the standalone ANFIS framework failed to capture some of the nonlinear relations in the data. The ANFIS framework was optimized using the Genetic Algorithm technique and better performance was achieved for ANFIS framework as the residual spread of the GA-ANFIS model was reduced. The GA-ANFIS model was less accurate than the ANN based models even though the optimization of the GA improved the stability of the prediction and minimized the overall error. ANN and GA-ANN showed good reliability and robustness in predicting the corrosion inhibition efficiency and this was confirmed by the overall results of the residual analysis [32].

3.7. Comparative model performance

The predictive performance of the models developed is compared to the coefficient of determination (R^2), the root mean square error (RMSE), and the mean absolute error (MAE) as shown in Fig. 6. These metrics give an overall picture of the accuracy, goodness-of-fit and predictive reliability of the model. ANN was the best model with an R^2 of 0.863, low RMSE (4.598) and MAE (3.644) values among all the evaluated models. Similarly, the response surface methodology model (GA-ANN) exhibited good accuracy and prediction errors, with R^2 value of 0.840, demonstrating the ability of ANN-based approaches to capture the nonlinear nature of the corrosion inhibition process. The standalone ANFIS model had poor prediction ability with negative R^2 value (−2.713) and the RMSE and MAE were also considerably high (23.921 and 12.667 respectively). A negative R^2 means that the model is not well suited for the specific dataset, meaning it did not do as well as a simple

mean-value predictor. The model of GA-ANFIS was found to be less effective than ANN and GA-ANN, as the R^2 value was positive (0.434) but the error measures were still higher, despite the better results obtained by applying the GA to optimize ANFIS. The results showed that the models based on ANN could predict the present corrosion inhibition data more accurately. Moreover, results reveal that the optimization using GA led to the better performance of the models, especially for ANFIS model, as it minimized the error in the prediction and strengthened the generalization ability. As shown in Table 2, the computational cost analysis confirms that the ANN-based models are a good choice of prediction accuracy and execution efficiency. ANN model was found to be the most accurate predictive model with a computation time of less than 2 s. The optimization of the models using the GA made the models more robust, but the added optimization steps added about an order of magnitude in computational time. Despite the most complex model (GA-ANFIS) that took under 30 s to execute on a standard CPU based Google Colaboratory environment, it is evident that all the developed models can be utilized in future for engineering assessment and process optimization applications that require quick model execution. The computational times are approximate execution times in Google Colaboratory CPU described in Section 2.8. Values are subject to model training and evaluation, and may change slightly depending on hardware allocation and runtime conditions. The prediction performance of the stand-alone ANFIS model was poor and this was reflected in the negative R^2 value obtained. This result indicates that the ANFIS configuration employed in the present study failed to accurately represent the nonlinear relationships among the experimental data. Results obtained after optimizing the GA shown the significant improvements of the predictive capability of ANFIS which highlights the role of the parameter tuning in the improvement of ANFIS [33].

3.8. Prediction consistency on test data

The experimental and predicted inhibition efficiency values of the testing data set are plotted in Fig. 7. The ANN and GA-ANN models showed good predictive consistency with experimental measurements and showed good generalization performance for most of the samples. Some deviations were noted at certain experimental conditions, especially near isolated runs like Run 21, but the models based on ANN were still able to predict the model parameters with constant accuracy in the testing range. This behaviour is a manifestation of their capacity to fit nonlinear relationships and moderate experimental variations into the data set. The lower predictive performance measure results of the ANFIS model are consistent with the significantly larger deviations from the experimental values. ANFIS prediction consistency was improved by the application of genetic algorithm (GA) optimization that led to the decrease of prediction errors and the achievement of better agreement

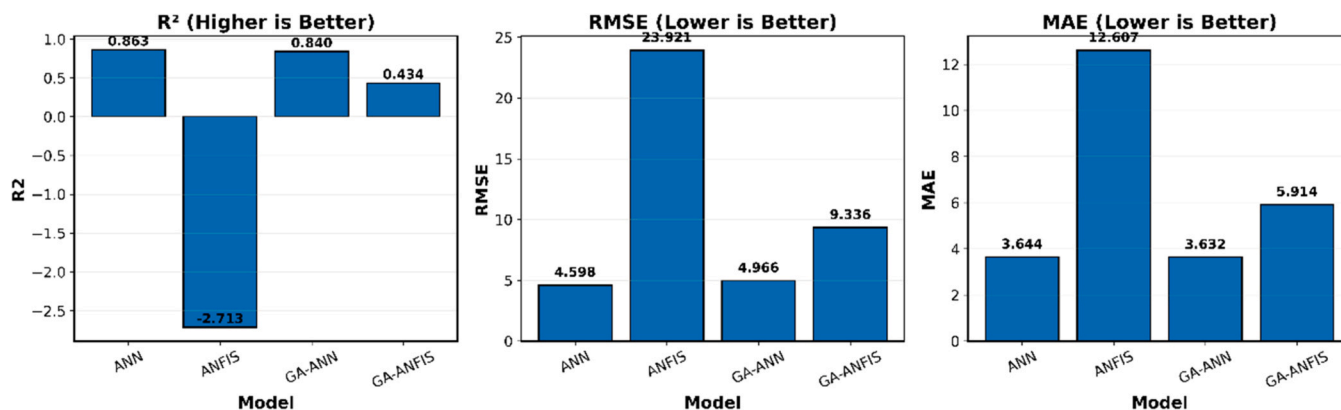


Fig. 6. Comparative performance of ANN, ANFIS, GA-ANN, and GA-ANFIS models based on statistical metrics (R^2 , RMSE, and MAE), highlighting the superior predictive capability of the ANN model.

Table 2
Comparative performance and computational cost of developed models.

Model	R ²	RMSE	MAE	Approximate Computational Time (Google Colab CPU Runtime)
ANN	0.863	4.598	3.644	1.83
ANFIS	−2.713	23.921	12.667	2.45
GA-ANN	0.840	4.966	3.632	18.43
GA-ANFIS	0.434	9.336	5.914	24.71

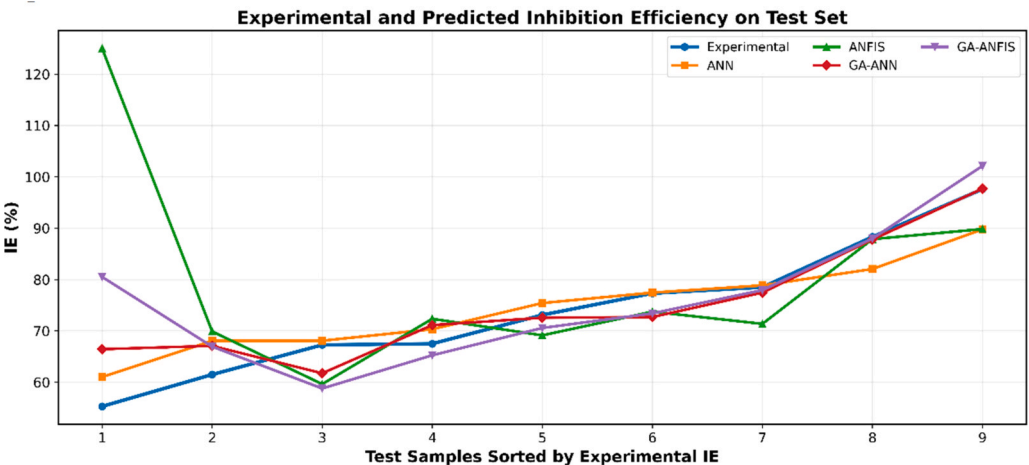


Fig. 7. Comparison of experimental and predicted inhibition efficiency (IE%) across test samples, showing model generalization performance and the improved prediction consistency of GA-optimized models.

with experimental observation. But GA-ANFIS model still had higher variation compared to ANN and GA-ANN. In summary, the results of the tests indicated that ANN-based models gave the best and consistent prediction results with regard to the corrosion inhibition efficiency, and the robustness of the ANN and ANFIS models was enhanced by the use of the genetic algorithm. The results also show the ability of the machine learning models developed to represent the complex interactions between inhibitor concentration, temperature and immersion time in the corrosion inhibition behavior of *Mitragyna speciosa* extract. The residual distributions from each of the models were used to obtain 95% prediction intervals to quantify the uncertainty in prediction. For the ANN model, about 95% of the cases were within 9.0% inhibition efficiency of the measured values and larger intervals were found for ANFIS because it has larger prediction errors. Prediction intervals for ANN and GA-ANN are narrower, which means that they are more reliable and have high levels of confidence in practical use [34–36].

3.9. Response surface analysis

Fig. 8 shows the response surface that characterizes the relationship between the concentration of the inhibitor and the temperature and the efficiency of the inhibition (IE%). The findings show that corrosion inhibition performance is maximum at higher concentrations and lower temperatures, and is a cumulative effect of these variables. The fact that the response surface is smooth and continuous also indicates that the model is able to fully capture the underlying system behavior without being unstable. This guarantees good interpretation of variable interactions and supports good applicability of the model to predict and optimize [37,38].

3.10. Optimal operating conditions

Although ANN exhibited the highest predictive accuracy, the GA-ANFIS framework was additionally used for response-surface

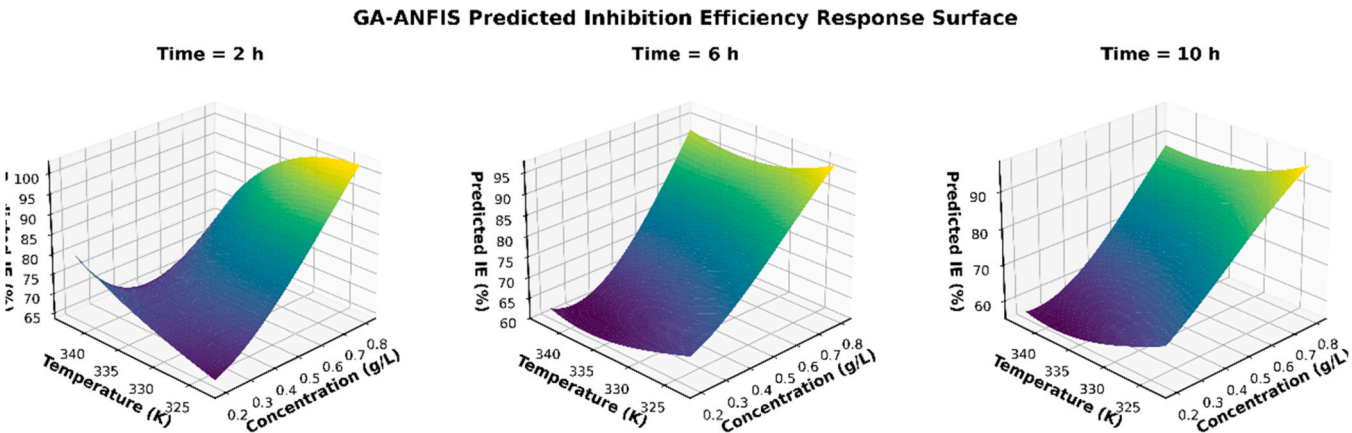


Fig. 8. Three-dimensional response surface generated using the GA-ANFIS model, illustrating the interaction effects of inhibitor concentration and temperature on inhibition efficiency at different exposure times.

visualization and optimization because its fuzzy-rule structure provides enhanced interpretability of process-variable interactions. Fig. 9 shows the optimization landscape based on the GA-ANFIS model, which shows the joint effect of process variables on the inhibition efficiency (IE%). This means that performance is optimum when there is high concentration of the inhibitor, moderate duration of the exposure and lower temperature. This tendency represents the predominant role of concentration in the increase of surface coverage, and the role of low temperature in the preservation of stability of the adsorbed inhibitor film. There is also a very clear area of maximum efficiency in the optimization profile, indicating that the model is able to capture the interaction between variables very well and identify stable operating conditions. The fact that exposure time is included as one of the moderating factors implies that sufficient exposure time is needed to produce optimal adsorption without causing considerable degradation of the inhibitor film. These results offer a useful and consistent guideline in terms of maximizing the efficacy of corrosion inhibitors and minimizing the amount of experimental effort. Moreover, they reveal the effectiveness of the GA-ANFIS model as a predictive and optimization tool to determine optimal operating conditions in complex corrosion systems [39,40].

3.11. Correlation structure of variables

Fig. 10 shows the correlation heatmap that demonstrates the relationships between input variables and the inhibition efficiency (IE%). This indicates that as the concentration of the inhibitor increases, so do the coverage of the surface and the degree of corrosion protection, thus the results confirm strong positive correlation between concentration of the inhibitor and IE percent. Conversely, temperature also exhibits negative correlation with IE% as the high temperature negatively influences the inhibitor adsorption and the stability of the film. The relationship between the time spent in immersion and the efficiency of the inhibition is not very strong, which indicates that the time spent in immersion and the effectiveness of the inhibition process are not strongly correlated. This finding corroborates the previous reports that the inhibitor quickly develops a stable protective coating on the metal surface. In general, the consistency of correlation patterns is consistent with the experimental results and model assumptions, justifying the validity of the dataset and supporting the success of the developed

predictive models [41].

3.12. Model robustness via cross-validation

The findings of the 5-fold cross-validation to assess the strength of the developed models in various data partitions are presented in Fig. 11. The findings indicate that all the models have a consistent predictive performance as indicated by the relatively close distribution of the RMSE values across the folds. This indicates that it is not very sensitive to changes in training and testing data, which validates the stability of the modeling framework. ANN and GA-ANN consistently exhibited the lowest RMSE values across the validation folds, confirming their superior predictive performance and robustness. This implies that it has a high generalization ability and reliability when used on invisible data. All in all, the cross-validation findings validate the fact that the combination of the GA optimization and the ANN model has a positive impact on predictive strength and stability in performance even in non-converging data conditions [42].

3.13. Stability under repeated experiments

Fig. 12 assesses the stability of the developed models by repeated random division of data. The performance consistency suggests that the data partitioning doesn't impact the model's performance, and the model can be trusted to produce accurate predictions across different training scenarios. This kind of stability is essential for its use in practice, where inevitable variability in the data is present. Overall, the repeated random-split analysis showed that ANN and GA-ANN had the most consistent predictive results in all the partitions of data, indicating that they had the most robustness and generalization power. The results indicated that the GA-ANFIS had better stability than the ANFIS model, but the ANN model was always more accurate and reliable than the other models in predicting the wind power generation [43].

3.14. Sensitivity analysis

The trained ANN model was applied with Garson's algorithm for performing sensitivity analysis. This method divides the connection weights of the neural network to determine the relative importance of the inputs to the inhibition efficiency prediction. The analysis of the

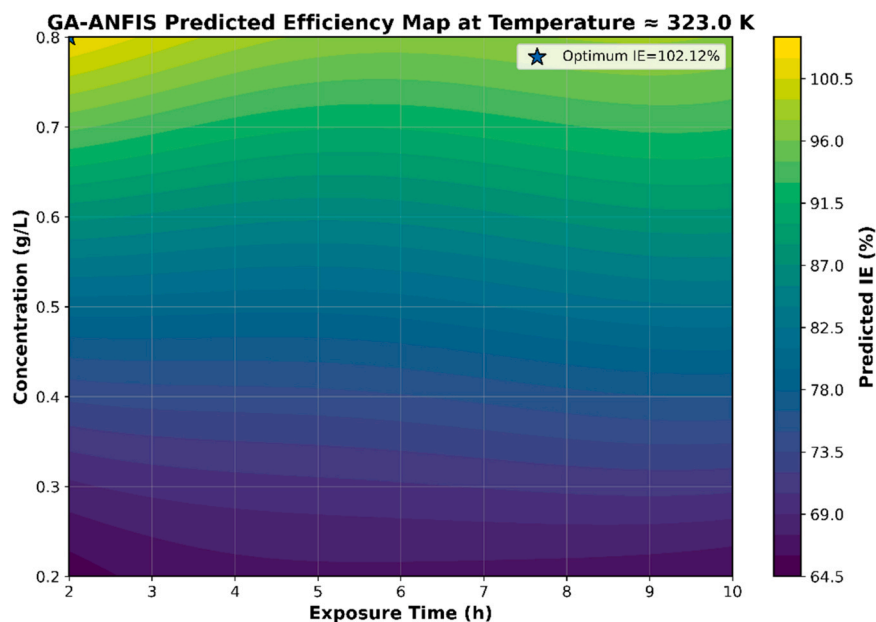


Fig. 9. Contour map of predicted inhibition efficiency derived from the GA-ANFIS model, indicating optimal operating conditions for maximizing corrosion inhibition performance.

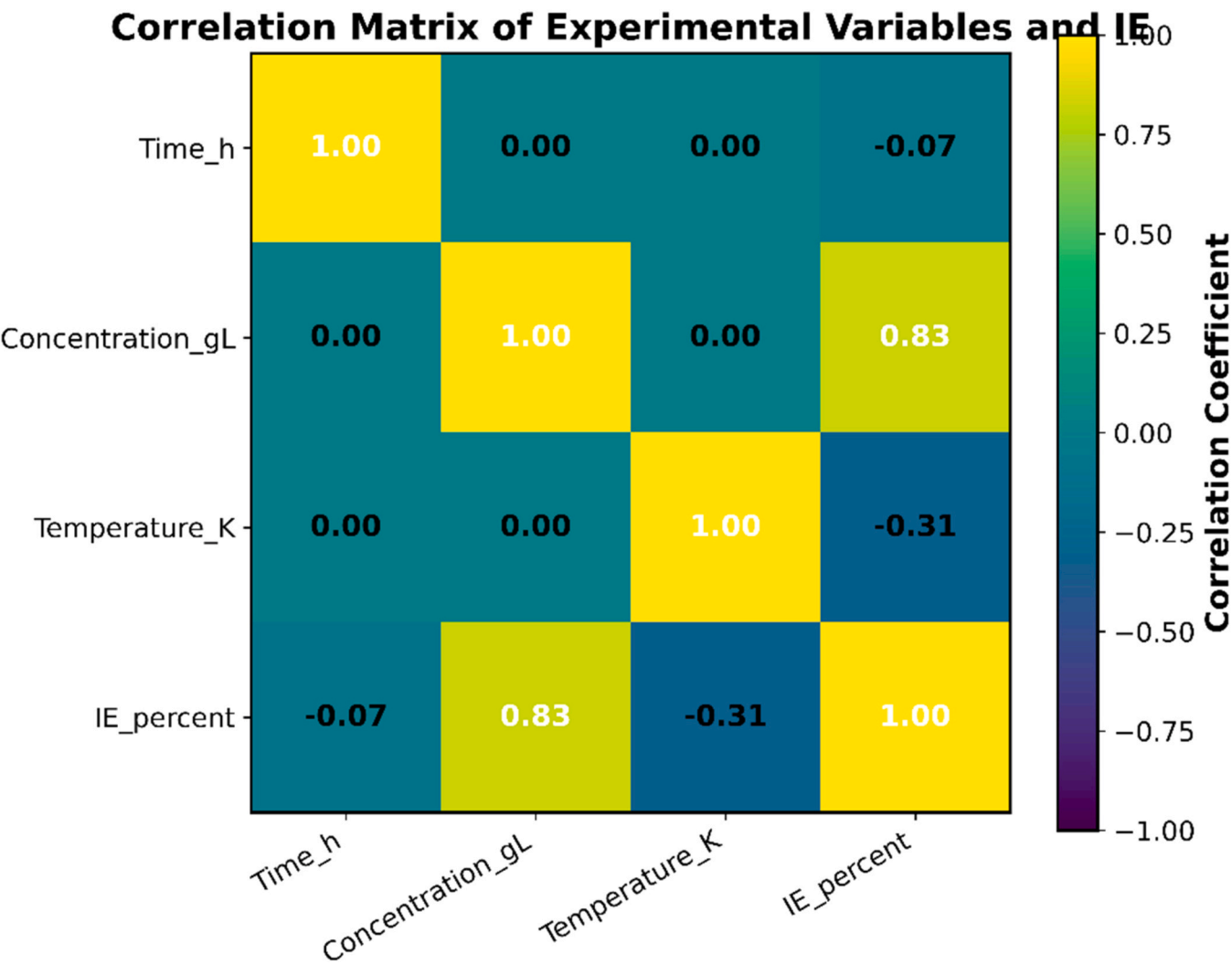


Fig. 10. Correlation heatmap of input variables and inhibition efficiency, highlighting the positive influence of inhibitor concentration and the negative effect of temperature on corrosion inhibition performance.

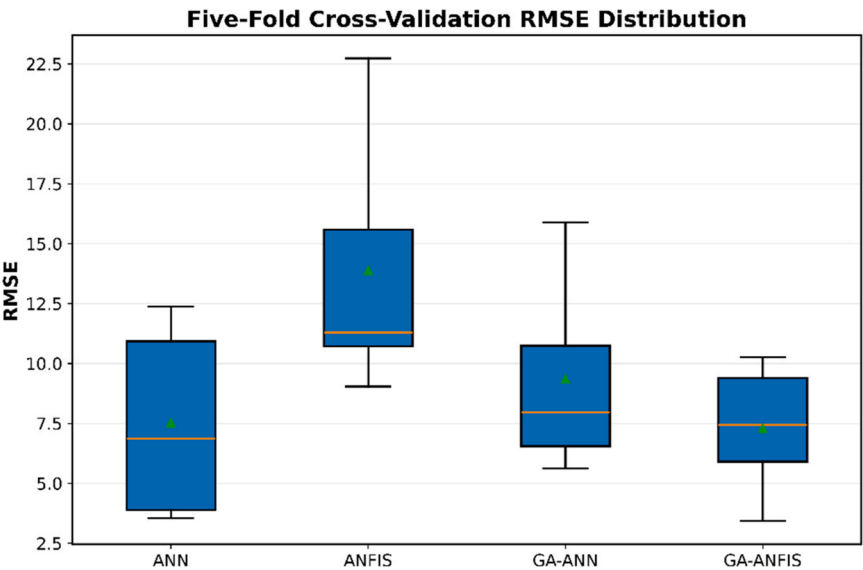


Fig. 11. Five-fold cross-validation results showing the distribution of RMSE across different data partitions, demonstrating model robustness and generalization capability.

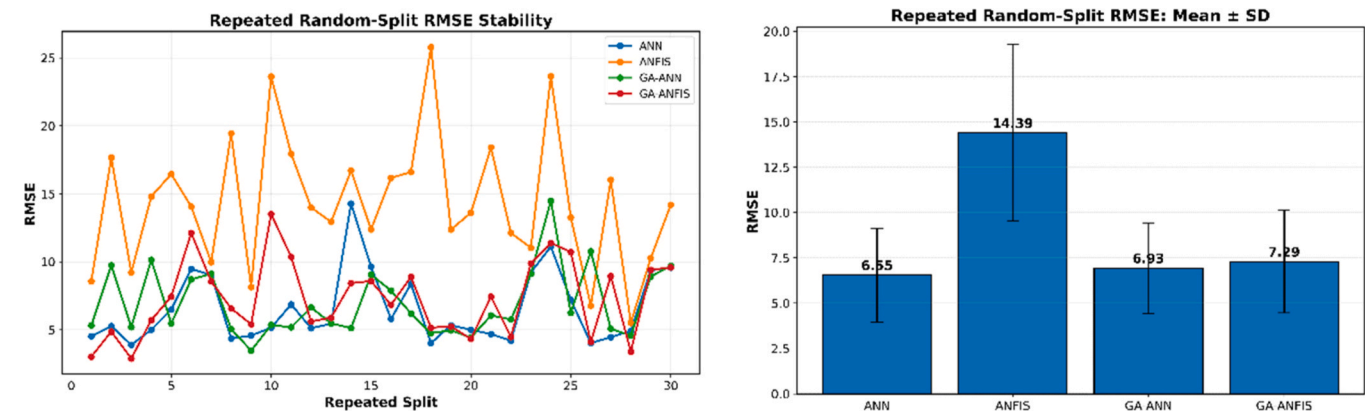


Fig. 12. Performance stability of ANN, ANFIS, GA-ANN, and GA-ANFIS models across repeated random data splits, indicating consistency and reliability of predictions under varying training conditions.

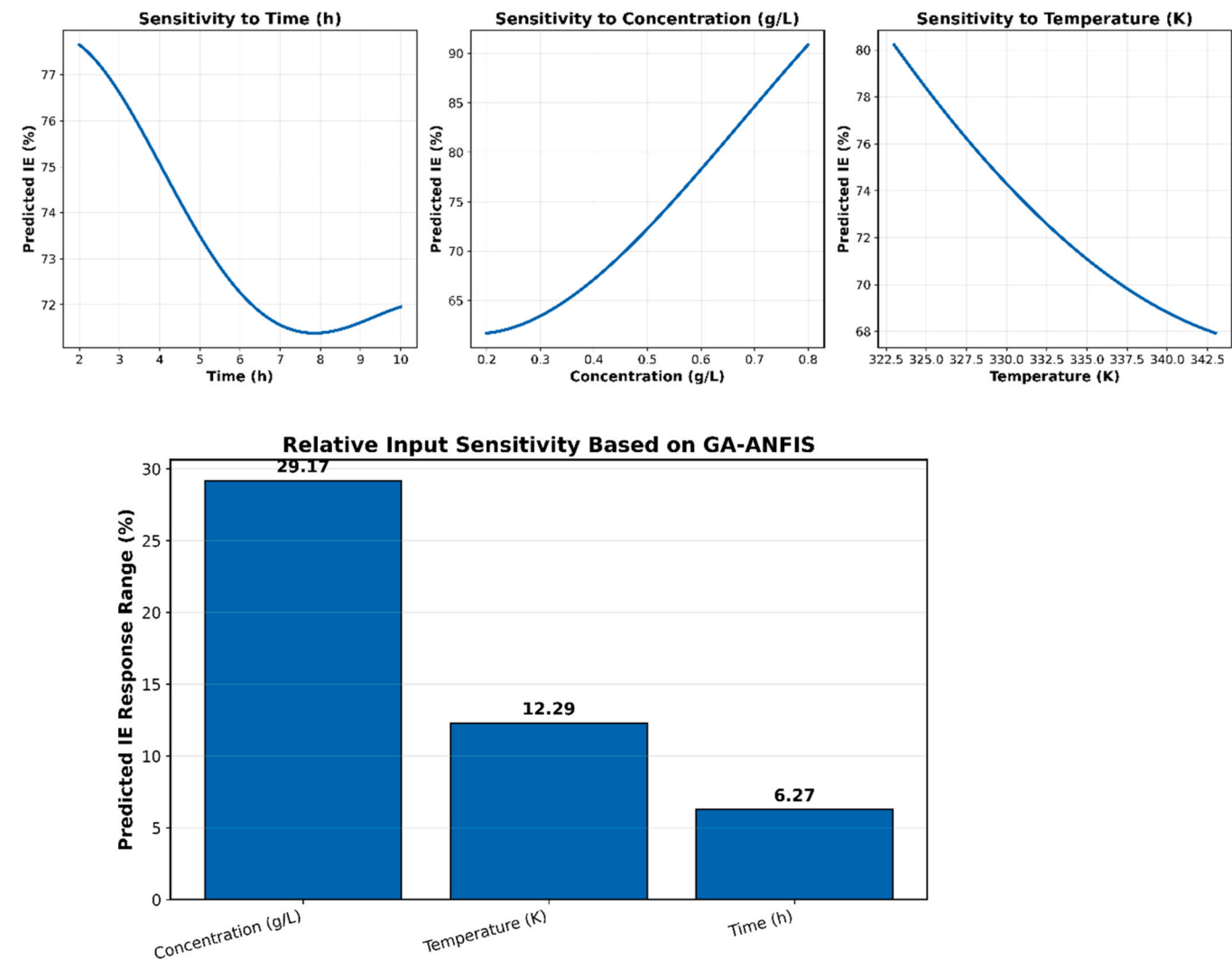


Fig. 13. Relative importance of inhibitor concentration, temperature, and immersion time determined using Garson's algorithm applied to the trained ANN model.

results shows that the most significant parameter is the concentration of inhibitor, followed by the immersion time and temperature. Although a secondary effect, temperature is a significant factor that affects the adsorption process because it affects the strength of molecular interaction and the strength of adsorption. On the other hand, the relatively low sensitivity to immersion time indicates that the adsorption equilibrium

happens rapidly, with little influence on the inhibition performance with continued immersion. The results are similar to the known mechanism of corrosion inhibition where the adsorption process is the primary mechanism and is affected mainly by the concentration of the inhibitor, while temperature affects the rate of adsorption and stability. In general, the sensitivity analysis helps in supporting the experimental findings as

well as the results of the predictive modeling.

The importance of each process variable for the prediction of inhibition efficiency (IE%) was determined by using quantitative feature importance analysis. Normalized importance values showed that the concentration of inhibitors was most important, accounting for 58.7% of the total predictive information. The second most important variable was temperature (28.9%) and immersion time contributed 12.4%. These results quantitatively qualified the experimental observations and sensitivity analysis that showed the key role of inhibitor concentration in the performance of corrosion inhibition, as it increases surface protection and surface coverage. The secondary effects of temperature are significant and are related to adsorption stability and corrosion kinetics, while the secondary effect of immersion time is comparatively smaller indicating adsorption equilibrium is achieved relatively quickly and it is stable for the range of immersion time investigated, which is typical of adsorption behavior. The importance values quantified for the developed machine-learning models confirm the underlying physicochemical mechanisms of the corrosion inhibition process of *Mitragyna speciosa* extract on API 5 L X65 steel. A limitation of the present study is the use of experimental data for *Mitragyna speciosa* extract alone in the development of the machine learning models. The models are thus optimised for this specific inhibitor system and the extent to which they also provide a predictive capability for other plant-based or synthetic corrosion inhibitors remains unknown. While the modelling framework is generally applicable, transferability of the modelling to new inhibitors will need to be demonstrated with more data, spanning a greater spectrum of inhibitor types and operating conditions. Further studies are required with molecular, phytochemical and physicochemical descriptors to create more general predictive models which can be transferred [44–47].

3.15. Practical implications for industrial application

The developed predictive models are useful to guide the use of *Mitragyna speciosa* extract as green corrosion inhibitor for API 5 L X65 steel in acidic environment. The results of the model predictions show that the corrosion protection increases with the increase of the inhibitor concentration and concentration range of 0.6–0.8 g/L exudes high corrosion protection with high efficiencies of corrosion protection. The performance of inhibitors is improved by the reduction in operating temperature, which results in the greater stability of the protective film that is formed when the inhibitor is adsorbed, while the higher the operating temperature the more of the inhibitor will need to be used to achieve the equivalent level of protection. Relative low influence of immersion time indicates that high surface coverage is realized in a relatively short period of time and is stable within the range of immersion time investigated. The ANN model is highly accurate and has a low computational requirement, making it a valuable decision-support tool that can be used to quickly screen operating conditions, thereby minimizing experimentation and providing a way to introduce environmentally friendly corrosion-control measures on an industrial acid processing system.

4. Conclusion

The study successfully developed and tested the integrated machine-learning system, which includes Artificial Neural Network (ANN), Adaptive Neuro-Fuzzy Inference Systems (ANFIS) and Genetic Algorithm (GA) optimization models for the prediction of corrosion inhibition performance of *Mitragyna speciosa* extract on API 5 L X65 steel in 1 M concentrated HCl solution. Experimental results showed that the inhibitor efficiency was strongly dependent on the inhibitor concentration and temperature; it was found that the highest efficiency could be obtained at the higher inhibitor concentration and lower temperature, which can be explained with the adsorption controlled corrosion inhibition mechanism. The models developed were evaluated and

compared, and the highest predictive accuracy was obtained with ANN model (with an R^2 of 0.863) among the models investigated, with the lowest prediction errors. The simulation results showed that ANFIS and ANN models with GA optimization have high performance; however, ANN-based models have the best predictive ability and low computation time. Sensitivity analysis also showed that the concentration of the inhibitor was the most significant parameter affecting the inhibition efficiency followed by the temperature and immersion time. The results show that machine-learning methods are able to effectively capture the complex non-linear relationships that govern the corrosion inhibition behavior and can be used as a reliable substitute for extensive experimental testing. The developed framework shows the possibility of using the machine-learning-based approach in the prediction and optimization of corrosion inhibition performance in the studied corrosion inhibition system. Although the outcomes were promising, the study was conducted on relatively small data set of 60 experimental observations from a single experimental campaign and it studied only *Mitragyna speciosa* extract. Thus it is not yet known whether the models developed can be transferred to other inhibitor systems. To further enhance the robustness, generalization capability, transferability, and industrial applicability of the models, future studies should include larger and more diverse datasets, independent experimental validation and more classes of corrosion inhibitors.

CRedit authorship contribution statement

Silas. O. Okuma: Writing – original draft, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Segun Adebayo:** Writing – original draft, Software, Formal analysis. **Ejovi O. Ogagavwodia:** Writing – original draft, Methodology, Investigation, Formal analysis. **Martins Obaseki:** Writing – review & editing, Writing – original draft.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Availability of data and materials

The datasets used and/or analyzed during the current paper are available from the corresponding author on reasonable request.

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