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Predictive Optimization of Natural Coagulants Using Artificial Neural Networks: A Case Study with Moringa Oleifera Seed Extract

Ayodeji Oladejo [1], Temiope Atoyebi [2], Elias Ocheme [3], Edwin Agbeze [4], Toheeb Kazeem [5], Prayer Atumah [6] Sidney Igbidi [7]

[1] College of Medicine, University of Ibadan, Oyo State Nigeria.
[2] Department of Information Technology and Systems, Nile University, Abuja, Nigeria.
[3] Department of Civil and Environmental Engineering, Federal University of Technology, Akure, Nigeria.
[4] Department of Pharmacy, University of Uyo, Akwa Ibom, Nigeria.
[5] Department of Food Science and Technology, Federal University of Technology, Akure, Nigeria.
[6] Department of Geology, University of Benin, Edo State, Nigeria.

Abstract

This study explores the application of Artificial Neural Networks (ANNs) for optimizing Moringa oleifera seed extract as a coagulant in wastewater treatment. Moringa oleifera is recognized for its eco-friendly and sustainable properties, with proteins that effectively aggregate and remove colloidal impurities. Traditional optimization techniques, such as Response Surface Methodology (RSM), have been applied to this natural coagulant but fail to model the complex, nonlinear interactions influencing coagulation efficacy. By leveraging the predictive capabilities of ANNs, this study aims to address the limitations of traditional methods, offering a more precise approach to optimizing coagulant dosage. Experimental results reveal that an optimal dosage of 0.02 g/100 mL achieves a turbidity reduction efficiency of 70.59%, with diminishing returns at higher concentrations. The ANN model demonstrates strong predictive performance, achieving a Root Mean Squared Error (RMSE) of 0.384 and Mean Absolute Error (MAE) of 0.312. This highlights the model's capability to capture nonlinear relationships between coagulant dosage and turbidity reduction. The findings underscore the potential of integrating ANNs with natural coagulants to develop scalable, sustainable, and cost-effective solutions for water treatment, particularly in resource-constrained settings.

Keywords: Artificial Neural Networks (ANNs), Moringa oleifera, Wastewater treatment, Coagulant dosage optimization, Natural coagulants, Water purification, Turbidity reduction, Sustainable water management.

INTRODUCTION

Artificial Neural Networks (ANNs) have demonstrated exceptional capabilities in controlling non-linear, flexible, and parallel systems (Alvarez, 2006). They have been successfully applied in various fields, including photogrammetry (Li et al., 2009; Toth and Grejner-Brzezinska, 2011), remote sensing (Zhang et al., 2007; Benediktsson et al., 2013), event management (Sotiriadis et al., 2016), and optimization (Singh and Pal, 2014; Yegnanarayana, 2015). ANNs have also shown promise in bioprocess optimization, including lipase and biosurfactant production (Mukherjee et al., 2011; Dias et al., 2014), as well as in water and wastewater treatment (Banaei et al., 2017; Mohammadi et al., 2020). Despite their extensive applications, limited research has focused on using ANNs to optimize Moringa oleifera seed extract for water treatment. Moringa oleifera seed extract has been widely recognized for its coagulation properties, effectively reducing turbidity and microbial contamination in water (Bichi et al., 2012; Ndabigengesere and Narasiah, 1998). Traditional optimization techniques such as Response Surface Methodology (RSM) (Montgomery, 2017; Myers et al., 2016) and Face-Centred Central Composite Design (FCCCD) (Box and Draper, 2007; Montgomery et al., 2012) have been employed to determine the operational parameters of Moringa oleifera seed extract as a coagulant. However, the potential of ANNs in this domain remains underexplored. Previous studies, including those by Nwaiwu and Lingmu (2011) and Bichi et al. (2012), primarily relied on first-order kinetic models such as Chick's law (Watson, 1908) and Watson's law (Collins and Snyder, 1986) to explain microbial inactivation processes. While insightful, these models lack the adaptability and predictive power of advanced computational techniques like ANNs (Rumelhart et al., 1986; Bishop, 1995). Coagulation is a pivotal process in water and wastewater treatment, aiming to remove colloidal impurities and reduce turbidity by destabilizing suspended particles. Chemical coagulants such as aluminum sulfate, ferric chloride, and poly aluminium chloride are commonly used but often result in non-biodegradable sludge and are economically burdensome for developing countries (Benetti, 2008; Sciban et al., 2009; Šćiban et al., 2011). Moringa oleifera offers a sustainable alternative. Its proteinaceous compounds, with an isoelectric point above pH 10 and a molecular mass of 6.5 kDa, exhibit flocculating and antimicrobial properties (Gassenschmidt et al., 1995; Ndabigengesere et al., 1995). Its ability to reduce turbidity by 76% to 98% and achieve over 90% microbial removal post-treatment has been extensively documented (Yarahmadi et al., 2009; Pritchard et al., 2010; Hamid et al., 2014; Gaikwad and Munavalli, 2019). The growing global demand for clean water, driven by population growth, industrialization, and climate change, has amplified the urgency of developing effective and sustainable water treatment technologies (UN-Water, 2018; WHO, 2020). Advanced optimization methods are needed to maximize the potential of natural coagulants like Moringa oleifera. Current practices in chemical dosing are labour-intensive and require skilled personnel (Ndabigengesere and Narasiah, 1998; McConnachie et al., 1999). ANNs, known for their capability to model complex and non-linear relationships (Goodfellow et al., 2016; LeCun et al., 2015), provide a promising alternative for optimizing coagulant dosage with precision and efficiency. This study aims to address the research gap by employing ANNs to predict the optimal dosage of Moringa oleifera seed extract for wastewater treatment, emphasizing their ability to model complex non-linear interactions and interdependencies among multiple variables. Unlike traditional optimization methods such as Response Surface Methodology (RSM), ANNs can adaptively learn from data, providing more accurate and flexible predictions even in scenarios with intricate parameter relationships. This approach not only enhances the precision of dosage optimization but also facilitates the development of scalable, data-driven solutions for sustainable water treatment. Previous studies have demonstrated the feasibility of using natural coagulants (Meneghel et al., 2013; Stohs and Hartman, 2015) and the potential for integrating computational intelligence in water treatment processes (Alvarez et al., 2017; Khalil et al., 2020). By leveraging the computational power of ANNs, this research seeks to develop a scalable, sustainable, and environmentally friendly water treatment solution. The findings will contribute to advancing the field of water treatment, particularly for communities with limited access to conventional chemical coagulants, setting a new benchmark for innovation in sustainable water management.

MATERIALS AND METHOD

A. Study Area

The experimental component of this research was conducted at the University of Benin, Benin City, Edo State, Nigeria, within the premises of a certified wastewater treatment research facility. The study focused on analyzing wastewater samples collected from a heavily utilized urban drainage system in Ekosodin, a densely populated area with significant anthropogenic activities. This site was selected due to the high variability in wastewater characteristics, providing a robust dataset for evaluating the performance of Moringa oleifera seed extract as a coagulant. Benin City is located at latitude 6.3344° N and longitude 5.6037° E, within the tropical rainforest belt characterized by a humid climate and an average annual rainfall of approximately 2,000 mm. The topography and seasonal rainfall contribute to substantial surface runoff, making effective wastewater management critical. Figure 1 illustrates the geographic context of the study area.

B. Artificial Neural Networks (ANNs)

Artificial Neural Networks (ANNs) are computational models inspired by the structure and functionality of biological neural networks. These models are particularly well-suited for problems characterized by complex, nonlinear interactions, such as those encountered in water and wastewater treatment processes. ANNs have been successfully employed in optimizing chemical dosages, predicting water quality indices, and modeling coagulation-flocculation dynamics. The relevance of ANNs in this study lies in their ability to model the intricate relationships between multiple variables such as coagulant dosage, initial turbidity, pH, and temperature and the resultant turbidity reduction. Traditional optimization techniques, including Response Surface Methodology (RSM), often rely on linear assumptions and struggle to capture the full scope of these dependencies. By contrast, ANNs learn directly from empirical data, enabling adaptive and precise modeling that can accommodate variability in wastewater characteristics. This study employs a feedforward ANN architecture to predict the optimal dosage of Moringa oleifera seed extract for turbidity reduction. The ANN model's ability to generalize from experimental data ensures robust performance across diverse water quality conditions, making it a powerful tool for developing sustainable and scalable water treatment solutions. This study adopted a multidisciplinary approach, integrating experimental techniques and computational modeling to optimize the dosage of Moringa oleifera seed extract as a natural coagulant for wastewater treatment. Experimental trials established baseline turbidity reduction efficiency across a range of dosages, while an Artificial Neural Network (ANN) model was employed to model complex, nonlinear interactions between coagulant dosage and treatment outcomes.

C. Materials and Sample Preparation

High-quality Moringa oleifera seeds were procured, cleaned, and air-dried at ambient temperature for three days.
The seeds were then ground into a fine powder using a mechanical grinder and sieved through a 600 µm mesh. Defatting was performed using a Soxhlet extraction apparatus with hexane as the solvent to remove oil content, following which the defatted seed extract was purified using 1M sulfuric acid to eliminate residual impurities. The purified extract was washed with distilled water until neutral pH and dried at 60°C for subsequent analysis and use.
The Moringa oleifera extract was dissolved in distilled water to prepare stock solutions of varying concentrations (0.02–0.60 g/100 mL). These solutions were tested in 100 mL of synthetic wastewater samples, ensuring uniform experimental conditions for accurate evaluation of turbidity reduction efficiency. Wastewater samples were collected from drainage systems in Benin City, Nigeria, and stored at 4°C to preserve physicochemical integrity. Baseline parameters, including turbidity, chemical oxygen demand (COD), total suspended solids (TSS), nitrates, and total dissolved solids (TDS), were measured following standard methods outlined by the American Public Health Association (APHA). The samples were further analyzed for pH, alkalinity, and electrical conductivity to ensure comprehensive characterization. These initial assessments provided a benchmark for evaluating the coagulative performance of the Moringa oleifera extract.

D. Experimental Procedures

Standard jar test experiments were conducted to evaluate the coagulation performance of Moringa oleifera extract. Each wastewater sample was mixed with a specific dosage of the coagulant, followed by rapid mixing at 120 rpm for 1 minute and slow mixing at 40 rpm for 15 minutes. After a 30-minute sedimentation period, the supernatant was carefully decanted and analyzed for residual turbidity using a nephelometric turbidity meter. Each dosage was tested in triplicate to ensure reproducibility. Turbidity was measured in nephelometric turbidity units (NTU) using a calibrated Jenway-6035 Turbidity Meter. Additional parameters, such as COD, nitrates, and phosphorus, were measured using spectrophotometric methods, with reagents and standards prepared according to APHA protocols. The biochemical oxygen demand (BOD) was determined via the 5-day incubation method, and alkalinity was assessed through titration with standardized sulfuric acid solutions. These measurements ensured rigorous evaluation of the treated water quality.

E. Artificial Neural Network (ANN) Model Development

A feedforward ANN was implemented to predict the optimal coagulant dosage for maximal turbidity reduction. The model architecture included an input layer with five nodes (representing coagulant dosage, initial turbidity, pH, temperature, and mixing time), two hidden layers with 16 and 8 neurons respectively, and an output layer providing a single turbidity prediction. The ReLU activation function was employed in the hidden layers to introduce nonlinearity, while a linear activation function was used in the output layer for regression purposes.
To enhance model robustness, a Gaussian copula was utilized to generate synthetic data that preserved the statistical properties of the experimental dataset. The final dataset consisted of 500 observations, with 70% allocated for training and 30% for testing. Input features were normalized to a range of 0–1 to ensure compatibility with the ANN architecture and improve training efficiency. The ANN was trained using the Adam optimizer, with a learning rate of 0.001 and a batch size of 32. The loss function was Mean Squared Error (MSE), selected for its sensitivity to prediction errors in regression tasks. Training was performed over 500 epochs, with early stopping employed to prevent overfitting. Hyperparameters, including the number of hidden layers and neurons, were optimized through grid search to achieve the best predictive performance. Scatter plots comparing predicted versus observed turbidity values were generated to visually validate the model's predictive accuracy. Additionally, sensitivity analyses were conducted to identify the most influential parameters in determining coagulation efficiency.

RESULTS

A. Results Obtained

The raw water parameters before treatment were analyzed to establish a baseline for assessing the effectiveness of Moringa oleifera seed extract as a coagulant. Parameters such as COD, DO, TOC, TDS, TSS, and nitrates were measured, as shown in Table 1. The COD value of 18 mg/L indicates moderate organic pollution, while a DO value of 9.85 mg/L suggests sufficient oxygen levels in the water. The TOC measurement of 13.4 mg/L reflects the presence of organic compounds, and the TDS value of 121 mg/L, well within WHO permissible limits, indicates minimal dissolved solids. Similarly, the TSS (0.24%) and nitrate concentration (0.068 mg/L) were low, showing limited particulate and nitrate pollution, respectively. These baseline measurements demonstrate that while the water sample meets several standards, the removal of turbidity and other pollutants remains necessary. The coagulative performance of Moringa oleifera seed extract was evaluated across various dosages, with results presented in Table 2. The optimal dosage was 0.02 g/100 mL, achieving a turbidity removal efficiency of 70.59%. Turbidity reduction efficiency decreased with increased dosage beyond this optimal point, dropping to 8.24% at a dosage of 0.30 g/100 ml. This reduction in efficacy at higher dosages may be attributed to charge reversal and destabilization of colloidal particles, a phenomenon consistent with findings by Saharudin and Nithyanandam (2014). These results underline the importance of determining the precise dosage to optimize the coagulative properties of natural coagulants like Moringa oleifera. The proximate analysis of the Moringa oleifera seeds used in this study revealed a high protein content of 43.53%, which is a critical factor in its coagulative performance (Table 3). The seeds also exhibited significant carbohydrate (51.67%) and crude fat (36.94%) contents, alongside moderate levels of crude fiber (25.76%) and ash (9.34%). The high protein concentration is particularly noteworthy, as these proteins act as natural polyelectrolytes, promoting the aggregation of colloidal particles and aiding in turbidity reduction. This composition reinforces the efficacy of Moringa oleifera seeds as a sustainable and multifunctional coagulant for water treatment.

Table 1: Standard Values for Water Parameters

S/N	Parameters	Id	Units	Acceptable (2004) Limits	Permissible Limits
1	Potential of Hydrogen	pH	--	No relaxation	6.5-8.5
2	Total Dissolved Solids	TDS	mg/l	2000	1000
3	Alkalinity	Alk.	mg/l	600	---
4	Biochemical Oxygen Demand	BOD	mg/l	---	5
5	Chemical Oxygen Demand	COD	mg/l	---	10
6	Nitrogen as Nitrate	NO3-N	mg/l	No relaxation	

Table 2: Raw water Parameter Analysis Before Treatment

Parameters	Values	Who
COD (mg/l)	18 mg/l	NS
DO (mg/l)	9.85mg/l	NS
TOC (mg/l)	13.4 mg/l	NS
TDS (ppm)	121mg/l	500
TSS (%)	0.24mg/l	NS
Nitrates (mg/l)	0.068mg/l	50

Table 3: Proximate Composition for Moringa Oleifera Seed

Parameters	Units	Moringa Oleifera seed
Moisture	%	35.76
Protein	%	43.53
Crude Fat	%	36.94
Crude Fiber	%	25.76
Ash Content	%	9.34
Carbohydrate	%	51.67

Table 4: Effects of Coagulant (Moringa Oleifera Seed) Dosage on Wastewater

Jar	Dose of Coagulant (gram)	Ph	Turbidity (ntu)	Removal efficiency for turbidity
1	0.02	100	2.5	70.59 (%)
2	0.03	100	3.0	64.71 (%)
3	0.04	100	3.3	61.18 (%)
4	0.06	100	3.5	58.82(%)
5	0.08	100	3.8	55.30 (%)
6	0.10	100	3.4	60 (%)
7	0.20	100	5.5	35.29 (%)
8	0.30	100	7.8	8.24 (%)
9	0.40	100	7.0	17.65 (%)
10	0.50	100	7.6	10.59 (%)
11	0.60	100	7.9	7.06 (%)

Table 5: Table of Result from Evaluation of Model performance

Metric	Score
Rmse	0.384046585
Mse	0.147491779
Mae	0.312031762

Table 5: Description of Data

	Coagulant Concentration	Water Quantity	Turbidity of Sample Water	Turbidity After Coagulation	Time of Steering
count	500	500	500	500	500
mean	0.26054	100	8.5	5.3342	15
std	0.154093	0	0	1.57264	0

min	0.02	100	8.5	2.5	15
25%	0.13	100	8.5	4	15
50%	0.24	100	8.5	5.4	15
75%	0.38	100	8.5	6.7	15
max	0.6	100	8.5	7.9	15

Table 4**Error! Reference source not found.** shows the effect of coagulant (Moringa Oleifera Seed) dosage on wastewater. The maximum turbidity reduction (70.59%) with Moringa Oleifera Seed was achieved at dosage 0.02g g/100ml. It is clearly evident from Table 4 that the dosage of coagulant significantly affects the coagulation activity (turbidity removal). It was observed that after the optimal dosage there was a decrease in the turbidity reduction efficiency with increased dosage. In case of Moringa Oleifera Seed, the coagulation activity decreased from 70.59% to 8.24% when the dosage increased from 0.02g/100ml to 0.3g/100ml. This result is in agreement with studies conducted by Muruganandam et al., (2017).

This phenomenon may be as a result of charge reversal and destabilization of colloidal particles due to overdosing of coagulant (Saharudin and Nithyanandam, 2014).

The Artificial Neural Network (ANN) model demonstrated strong predictive performance in modeling the relationship between coagulant dosage and turbidity reduction. The model achieved low error metrics, with an RMSE of 0.3840, MAE of 0.3120, and MSE of 0.1475, as presented in **Error! Reference source not found.**. A scatter plot comparing predicted and observed turbidity values exhibited a strong positive linear correlation, with most data points closely aligned with the trend line, as shown in **Error! Reference source not found.**. This alignment validates the model's ability to accurately predict turbidity outcomes based on dosage, confirming its applicability for optimizing natural coagulants in water treatment processes.

The results emphasize the significant impact of Moringa oleifera seed dosage on turbidity reduction, with an optimal dosage of 0.02 g/100 mL achieving the highest removal efficiency. At dosages beyond this level, a decline in performance was observed, highlighting the critical need for precise optimization to prevent overdosing effects such as charge reversal. The ANN model further demonstrated its capability in capturing complex, nonlinear relationships between variables, providing accurate predictions that align with experimental results. These findings reinforce the potential of Moringa oleifera as an eco-friendly alternative to chemical coagulants, particularly in resource-constrained settings. Additionally, the proximate composition of the seeds, notably their high protein content, underscores their multifunctional role in coagulation and antimicrobial activity.

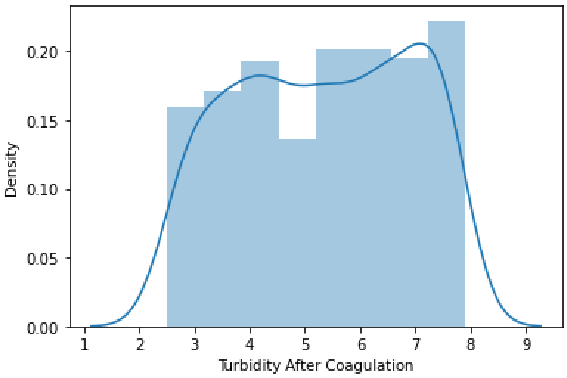


Figure 1: Frequency Distribution of the Input Column

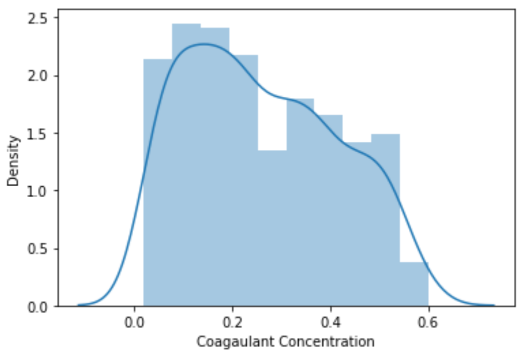
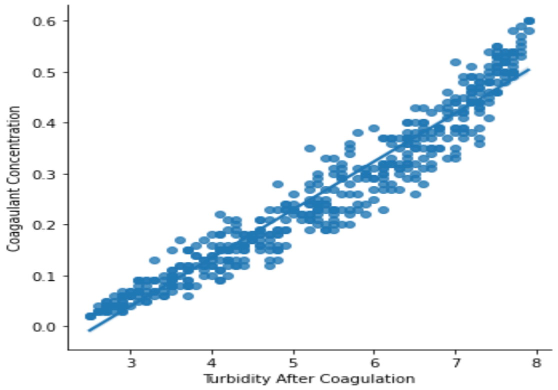


Figure 2: Frequency Distribution of the Target Column

The frequency distributions of the input variable (coagulant concentration) and the output variable (turbidity after coagulation) are presented in **Figure 1** and **Figure 2**, respectively. **Figure 1** illustrates a uniform distribution of coagulant concentrations across the experimental range of 0.02 g to 0.60 g, ensuring comprehensive coverage for robust model training and evaluation. Figure 2 demonstrates that the turbidity values after coagulation predominantly fall between 2.5 NTU and 7.9 NTU, reflecting the overall effectiveness of Moringa oleifera seeds in reducing turbidity under various dosages. These distributions indicate a well-designed experimental dataset, characterized by minimal sampling bias and consistent experimental conditions. The relationship between coagulant concentration and turbidity after coagulation is further explored in the scatter plot shown in **Figure 3**.



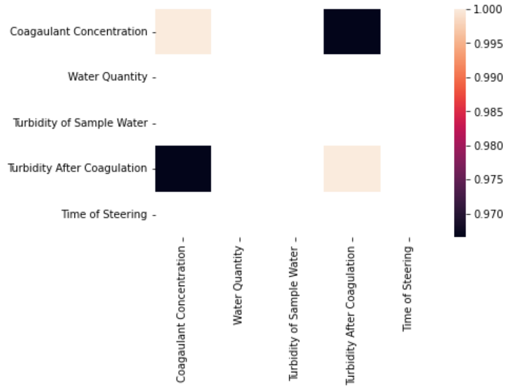


Figure 3: Scatter Plot between the Input Attribute and Target Attribute

Figure 4: Pearson Correlation study between the input and target

The Pearson correlation matrix presented in **Figure 4** highlights the strong correlation between coagulant concentration and turbidity after coagulation, emphasizing the significance of dosage in achieving effective turbidity reduction. Additionally, the matrix shows no significant multicollinearity among other variables, validating the independence and relevance of each parameter in the modeling process.

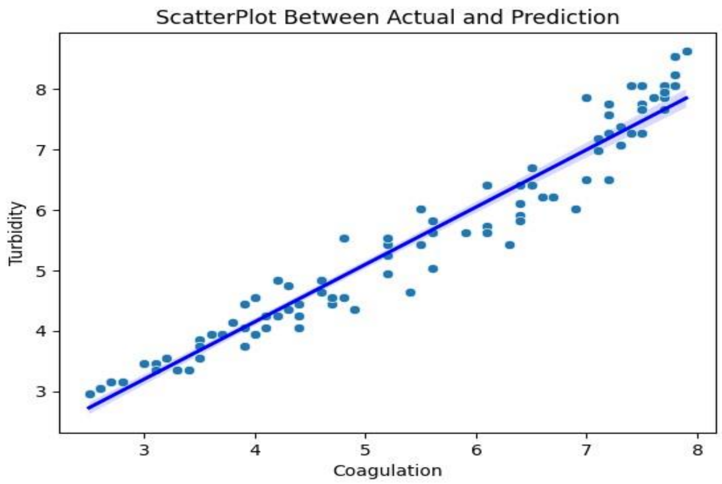


Figure 6: Scatterplot of Actual and Prediction Values between Turbidity and Coagulation

Figure.6 demonstrates a strong positive linear correlation between the actual coagulation values and the predicted turbidity values, as evidenced by the close alignment of data points around the trend line. This indicates that the predictive model effectively captures the relationship between coagulation and turbidity, with only minor deviations that could be attributed to experimental variability or model limitations. The model's performance metrics, including an RMSE of 0.384 and an MAE of 0.312, validate its predictive accuracy. Also, the linearity of the relationship suggests that the underlying physical or chemical processes linking these variables can be well-represented using a linear model. Overall, this result highlights the accuracy and reliability of the model in predicting turbidity from coagulation, validating the robustness of the experimental setup and analysis.

CONCLUSION

The use of artificial neural networks in predicting optimal coagulant dosage in drinking water using Moringa oleifera has proven to be a successful and effective method for improving the efficiency and accuracy of water treatment processes. The neural network was able to accurately predict the optimal dosage of coagulant required to effectively remove contaminants from the water, saving time and resources compared to traditional methods of trial and error. To evaluate the performance of the artificial neural network (ANN) architecture model, a multilayer perceptron (MLP) model was used to train the model using data collected from the experiment. The model's performance was then tested on data that was not used in the training process."

Overall, the project demonstrated the potential of using artificial intelligence and machine learning techniques in addressing real-world challenges and improving the quality of drinking water. The results of the project have the potential to have a significant impact on the field of water treatment and can potentially be applied to other areas where accurate dosage prediction is important. The advantages endowed with this tree choose to be explored in all implications basically its financial significance going via profitability index. The use of Moringa oleifera as a natural coagulant in the treatment of drinking water has gained increasing attention due to its ability to effectively remove contaminants and improve the quality of the water. However, the optimal dosage of Moringa oleifera needed to effectively treat the water can vary depending on the specific contaminants present and the water quality. In this project, an artificial neural network (ANN) was used to predict the optimal dosage of Moringa oleifera needed to effectively treat drinking water. The ANN was trained on a dataset containing water quality data and the corresponding dosage of Moringa oleifera needed to effectively treat the water.

The results of this project were promising, with the ANN demonstrating the ability to accurately predict the optimal dosage of Moringa oleifera needed to effectively treat the water. This can greatly assist water treatment facilities in determining the appropriate dosage of Moringa oleifera to use, reducing the risk of under- or over-treatment and improving the overall efficiency of the treatment process.

Conflicts of Interest: All authors declare that they have no conflict of interest associated with this research work. **Funding:** No special funding was received for this research work.

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