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(RESEARCH ARTICLE)

Artificial neural network modelling of cyanide transport in a soil contaminated with cassava wastewater

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Abstract

Understanding the transport of cyanide present in cassava wastewater is very crucial especially when choosing the right remediation technique to employ to restore the soil's fertility. In this study, the concentrations of cyanide for both dry and wet seasons were determined on two sites of area (2.5 m by 2.5 m) respectively. Physico-chemical characterizations were carried out on the soil samples collected. Using the artificial neural network (ANN) approach for this study, a total of 91 samples were used for each season which were divided into 63 samples for training, 15 samples for validation, and 15 samples for testing. Three input parameters consisting of (depth, time, and measured concentration) were used to obtain one output parameter (predicted concentration). The performance of the ANN model was evaluated using metrics such as MSE, RMSE, R, and R^2. The results showed that ANN model was able to predict the concentration of cyanide for both seasons as evident in their MSE and RMSE values close to zero and the R^2 values close to unity. However, the data set for dry season had better ANN predictability than that of the wet season as shown by the R^2 values for the training, validation and testing of the dry season to be 0.9954, 0.9978, and 0.9942, while the wet season is 0.9944, 0.7887 and 0.7793 respectively. Therefore, ANN model could be used to predict the concentration of cyanide at varying depths and times.

Keywords: Cyanide; Cassava Wastewater; Artificial Neural Network (ANN); Prediction; Transport

1. Introduction

Nigeria is the largest producer of cassava with approximately 45 million tonnes in 2009, which was almost 19% of production in the world [1]. This may be due to its low cost of production and wide range of uses as evident in products like garri, fufu, tapioca, starch, akpu and other more products [2, 3]. In the course of producing these food, a lot of wastes are generated of which wastewater is inclusive. The demand for cassava is becoming increasingly high by the day and has also led to increase in environmental pollution with regard to the disposal of the effluents [4]. For instance, in the processing of cassava to garri or fufu, a large amount of water is used, which in turn leads to the discharge of a large amount of wastewater [5].

The indiscriminate discharge of cassava wastewater produced offensive odours and unsightly scenarios and its discharge on the soil had affected the soil and groundwater, including biota (plants and micro-organisms) within the environs of the mill [6, 7].

Cassava and its wastewater had been reported to be toxic and poisonous [8-11]. This toxicity was as a result of its pH and cyanide content. Nok and Ikediobi [12] reported that the pH of fermenting cassava was between 5.5 and 6.3. In other words, disposal of large amount of cassava wastewater had made the soil pH to be too acidic and caused plant not to utilize N.P.K and other nutrients [13], and had led to plant uptake of toxic metals which may eventually had led to

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death [14]. Osunbitan [15] carried out chemical analysis on the cassava wastewater and studied its effect on some of the soil exchangeable cations with regards to depths of 10 to 50 cm. Olukanni *et al.* [16] also investigated on the interaction between the suspended solids and settled solids of cassava wastewater by monitoring parameters such as pH, cyanide, coliform, biochemical oxygen demand (BOD) and suspended solids (SS).

Others had also done microbial and physicochemical analyses on soils contaminated with cassava wastewater and the results had shown that cassava wastewater had a negative effect on soil microbial characteristics, physicochemical properties and low microbial and fungi load in the soil [17-22].

The numeracy of literatures on the effect of cassava on the soil's physicochemical properties as well as microbial activities is no doubt high. However, cyanide movement in soil and its potential to contaminate groundwater have not been fully reported. Also, several researchers had applied various analytical and numerical models on the flow of water and other contaminants but not with cassava wastewater [23-30]. For instance, the conventional one-dimensional convection dispersion equation (CDE) had been used to describe solute transport in the soil [31-34]. These models used fixed transport parameters for the CDE which are only valid for homogenous medium or laboratory scale but not for heterogeneous field scale. As an alternative, stochastic transfer functions were introduced to describe the transport of solutes in the soil but this follows the 'Black box' concept that is based on a linear relationship between inputs and outputs. Additionally, this only gives a representation of solute transport in soil but not the physical transport processes [35-37].

In recent times, many researchers have applied artificial neural network (ANN) to predict hydraulic properties [38,39] such as saturated hydraulic conductivity [40-45] and soil water retention [45-48] but few have employed ANN in predicting the concentration of contaminants or its breakthrough curves as well as solute transport parameters [49-60]. Hence, the need to apply ANN to predict cyanide concentration over long distances and/or time periods. Therefore, this paper focuses on applying artificial neural network (ANN) in predicting cyanide transport in a soil contaminated with cassava wastewater. It will also compare the ANN model performance for both dry and wet seasons using performance metrics like mean square error (MSE), root mean square error (RMSE) and correlation coefficient (R^2).

2. Material and method

2.1. Experimental setup

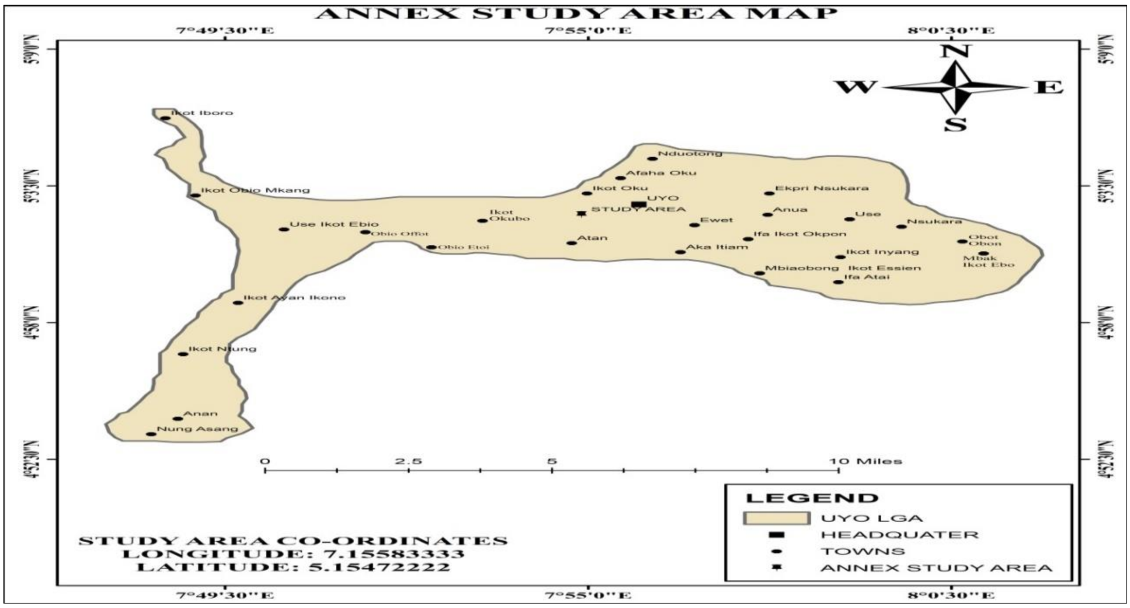

Figure 1 Coordinate site description for dry season

Two sites were used for the transport studies of cassava wastewater in soil. One for dry season while the other was for wet season. The dry season site used was the Research farm area belonging to Faculty of Agriculture, University of Uyo, Annex Campus. This area had been used by internship students for cultivating several crops and this had been done over the years. The site coordinates were 05° 02' 26.3" N, 007° 55' 16.8" E and 2.14 ft elevation. The site used for rainy/wet season was a plot beside Faculty of Agriculture, University of Uyo, Main Campus. Its coordinates were 05° 02'40.9" N, 007° 58' 42.3" E, and elevation of 133 ft (see Figure 1 and Figure 2).

At both sites, 500 litres of cassava wastewater was poured on a field site area of 2.5 m by 2.5 m. However, on pouring the cassava wastewater and allowing it to infiltrate completely, soil samples were collected randomly at four points using an auger for 7 depths of ranges of 15 cm intervals up to a depth of 120 cm (i.e 0-15, 15-30, 30-45, 45-60, 60-75, 75-90, and 90-120) and characterization of the samples were done in replicates at interval of 5 days for a period of two months [24].

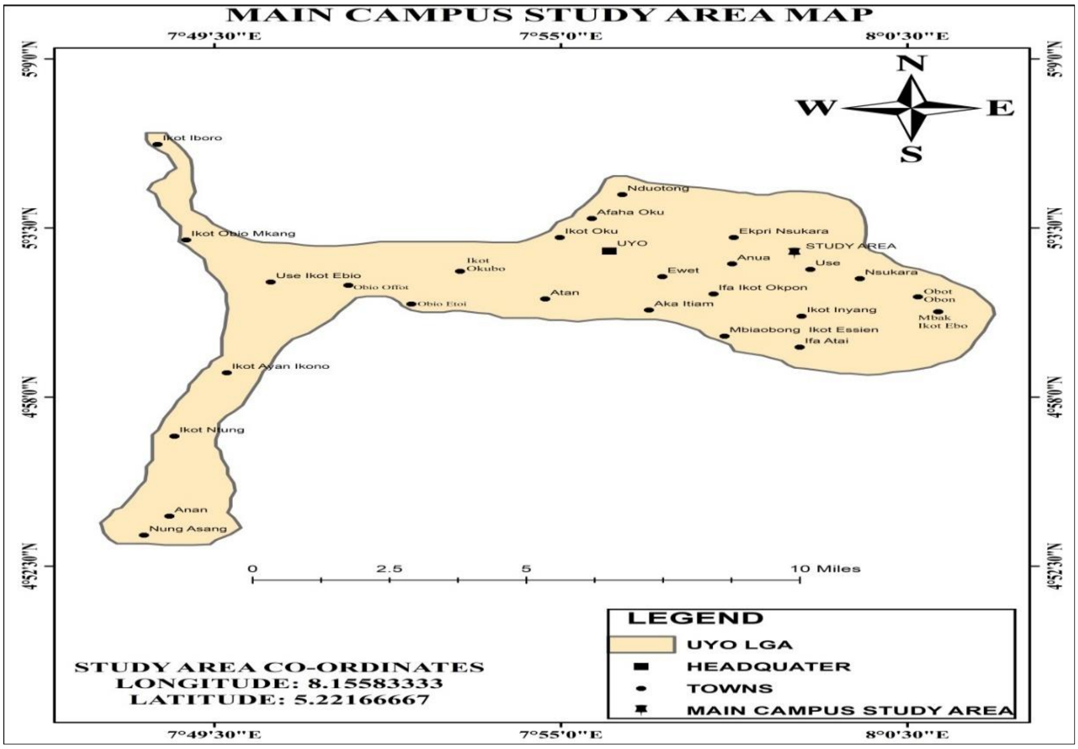

Figure 2 Coordinate site description for wet season

2.2. Data training setup

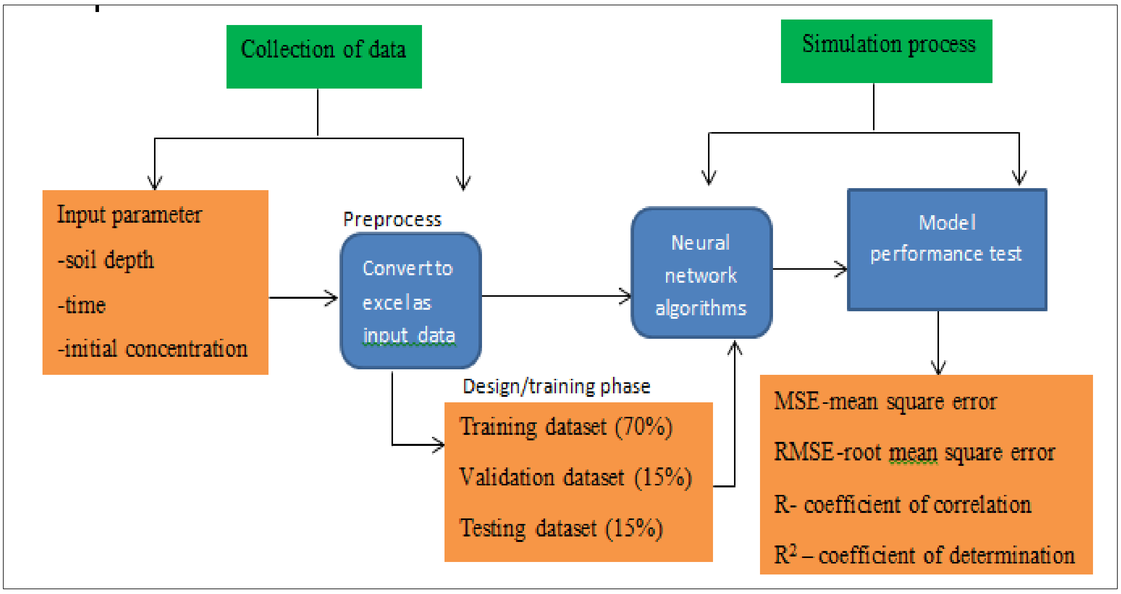

Figure 3 Schematic diagram of artificial neural network algorithm used for predicting the concentration of cyanide in the soil

In this study, neural network toolbox of MATLAB 2015a mathematical software was used to predict the concentration of cyanide for dry and wet seasons. The algorithm for this process is presented in Figure 3. A total of 91 samples for each seasons were used in the simulation process and were subjected to training by splitting the 91 samples into 70% training (63 samples), 15% validation (14 samples), and 15% test (14 samples) as presented in Table 1. Additionally, both seasons used three inputs data involving (time, depth, measured initial concentration) to obtain one output data (predicted concentration). In order to determine the optimal architecture for the networks, a trial-and-error approach was used to select the optimum number of neurons in the hidden layer. The weights and bias factors were adjusted till each input yields the desired output [61].

Table 1 Neural network input parameters for dry and wet seasons

Number of data samples		
Training	Validation	Testing
63	14	14

2.3. Model evaluation methods

The performance of the ANN model needs to be evaluated. Therefore, a statistically-based approach was designed to achieve this purpose. In this study, four statistical metrics- Pearson correlation coefficient (R), the square of the correlation coefficient (R^2), the mean square error (MSE), and the root mean square error (RMSE) were used. These metrics are further described mathematically using equations (3) – (6) [61,62].

$$R = \frac{\sum_{i=1}^{n}(A_i-\overline{A_i})(M_i-\overline{M_i})}{\sqrt{\sum_{i=1}^{n}(A_i-\overline{A_i})^2\sum_{i=1}^{n}(M_i-\overline{M_i})^2}} \tag{3}$$

$$R^2 = \left(\frac{\sum_{i=1}^{n}(A_i-\overline{A_i})(M_i-\overline{M_i})}{\sqrt{\sum_{i=1}^{n}(A_i-\overline{A_i})^2\sum_{i=1}^{n}(M_i-\overline{M_i})^2}}\right)^2 \tag{4}$$

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

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

Where n is the total number of training data samples, A_i is actual target value, and M_i is the estimated target value, $\overline{M_i}$ and $\overline{A_i}$ are the average values of the estimated and actual target values respectively.

3. Results and discussion

The statistical description of the input parameters for both seasons is presented in Table 2 and Table 3. The ANN training process for the dry season was truncated at 211 epochs for a 3-2-1 ANN architecture since it gave the best ANN prediction (see Figure 4a and Figure 5a). Thus, the 3-2-1 architecture was considered the best ANN for predicting cyanide transport in soil for dry season due to its high prediction capability. Whereas the wet season had the training process truncated at 141 epochs with a 3-3-1 ANN architecture (see Figure 4b and Figure 5b).

Table 2 Descriptive Statistics of the input parameters used in the ANN modeling for dry season

Parameter	**Minimum**	**Maximum**	**Range**	**Mean**	**Standard deviation**
Depth (m)	0.15	1.20	1.05	0.6214	0.3347
Time (day)	0	60	60	30	18.7083
Concentration (mg/100 g)	0.028	2.260	2.232	0.7162	0.5750

Table 3 Descriptive Statistics of the input parameters used in the ANN modeling for Wet season

Parameter	Minimum	Maximum	Range	Mean	Standard deviation
Depth (m)	0.15	1.20	1.05	0.6214	0.3347
Time (day)	0	60	60	30	18.7083
Concentration (mg/100 g)	0.138	3.463	3.325	0.7047	0.4862

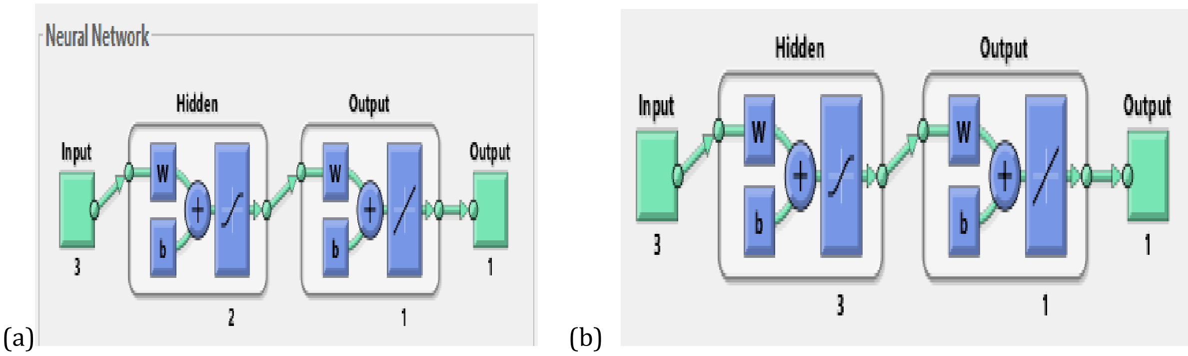

Figure 4 Optimum ANN model architectures (topology) for (a) dry season (b) wet season

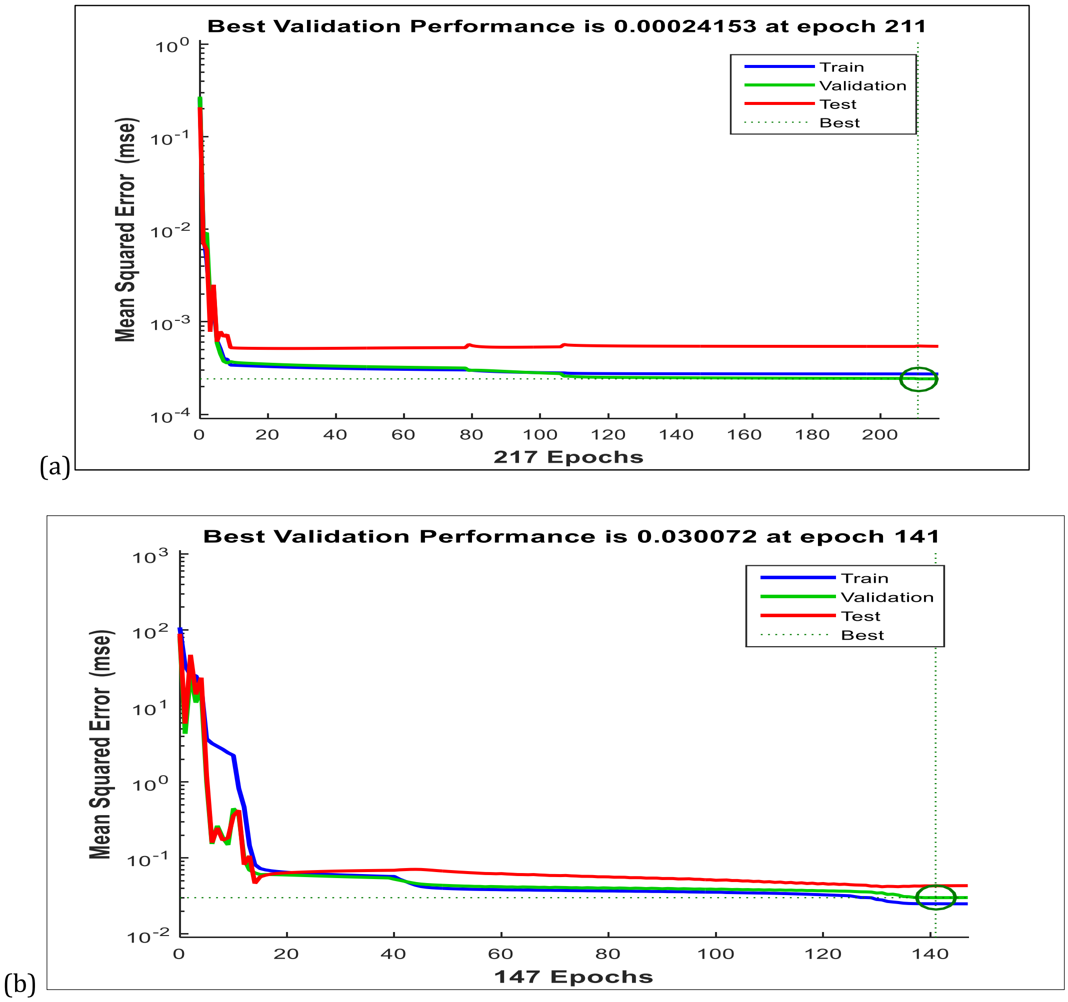

Figure 5 Performance plot of the developed ANN model for (a) dry season (b) wet season

The weights and biases of each season's ANN model are presented in Table 4 and Table 5, while the explicit model equations for each season are given in equations (7) – (9) respectively.

Table 4 Weights and biases for the model in dry season

IW			**b1**	**LW**	**b2**
-0.01767	0.235034	0.498366	2.091805	-11.5973	10.92603
-2.45792	4.641273	-15.0467	-12.1533	0.404589	

The explicit form of the model for predicting cyanide concentration in dry season is given by:

Denormalized model: $C = 2.232C_n + 0.028$ (7)

Normalized model

$C_n = A + B + 10.92603$ (8)

Where:

$A = -11.5973\tanh[-0.01767x + 0.235034t + 0.498366C_o + 2.091805]$ (8a)

$B = 0.404589\tanh[-2.45792x + 4.641273t - 15.0467C_o - 12.1533]$ (8b)

Where C is the predicted concentration, C_n is the normalized concentration, x is the depth, t is the time and C_o is the measured initial concentration.

Table 5 Weights and biases for the model in wet season

IW			**b1**	**LW**	**b2**
-4.99455	-1.06133	5.80974	-2.15581	1.450448	-1.82641
-0.04606	-0.54855	0.718681	-1.60167	-4.98819	
0.122237	2.070759	-0.04762	3.318265	-2.57808	

The explicit model for predicting cyanide concentration in wet season is shown below:

$Concentration\ (C) = A + B + C - 1.82641$ (9)

Where

$A = 1.450448tanh[-4.99455x - 1.06133t + 5.80974C_o - 2.15581]$ (9a)

$B = -4.98819tanh[-0.04606x - 0.54855t + 0.718681C_o - 1.60167]$ (9b)

$C = -2.57808tanh[0.122237x + 2.070759t - 0.04762C_o + 3.318265]$ (9c)

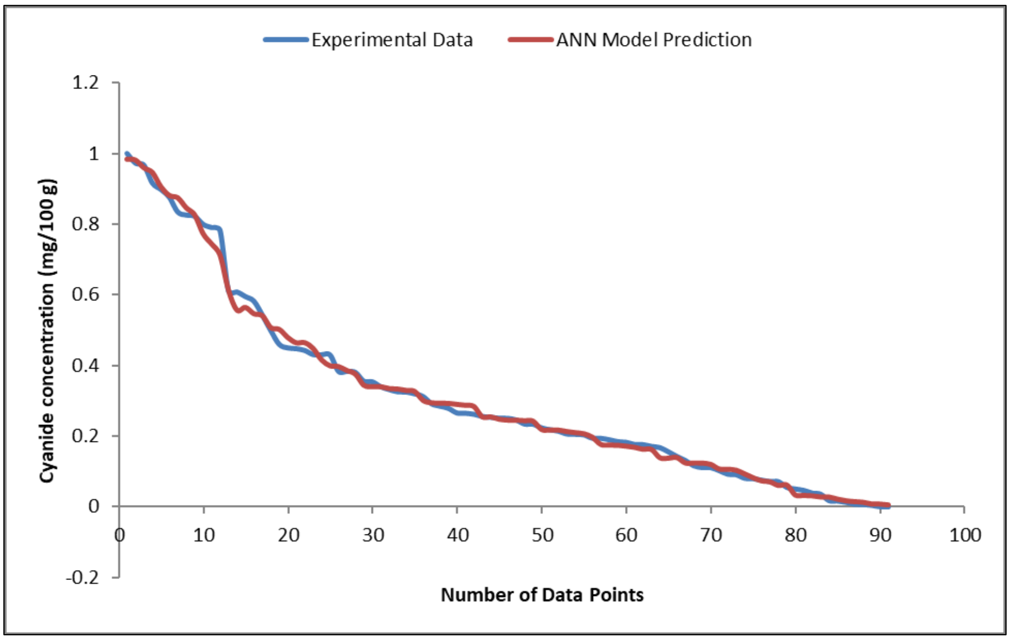

Figure 6 ANN prediction and Experimental values of cyanide concentration for dry season

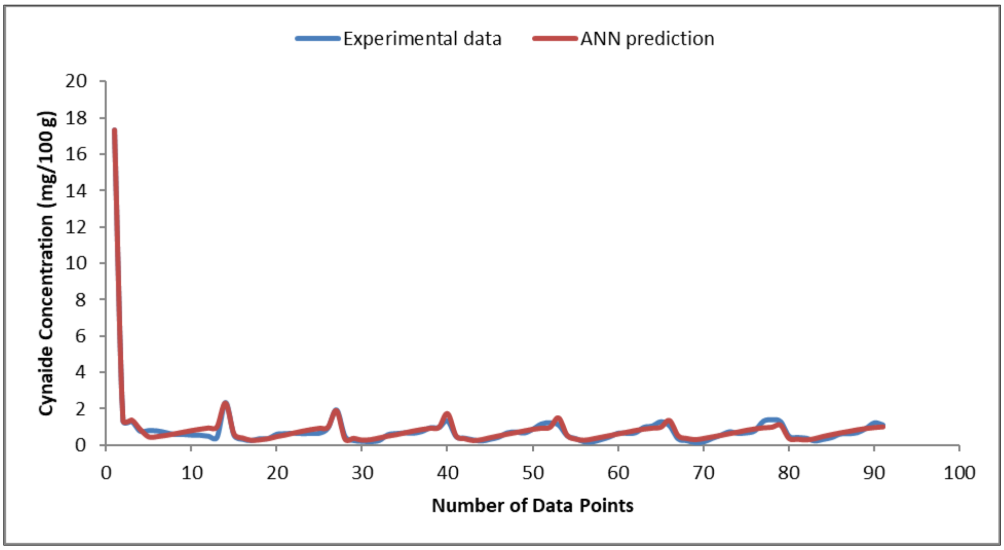

Figure 7 ANN prediction and Experimental values of cyanide concentration for wet season

Figure 6 and Figure 7 give the plots of cyanide concentration predicted by the ANN model and that of the experimental values for both dry and wet season. The results showed that both the ANN and experimental plots for both seasons are well matched and as such they are in good agreement.

A summary of the ANN model performance are presented in Table 6 and Table 7 for both dry and wet seasons. As shown in Table 6 and Table 7, the model performance metrics, MSE and RMSE values were lower for the training, validation and testing samples while R and R^2 values were higher. However, the dry season had a higher ANN predictability than that of the wet season as indicated by the R^2 values for the training, validation and testing of the dry season (0.9954, 0.9978, and 0.9942 respectively) to be close to unity. Whereas, the wet season had only the R^2 value for the training samples (0.9944) to be close to unity while the validation and testing samples had the R^2 values (0.7887 and 0.7793 respectively) to be lower a bit. This shows that ANN was able to predict cyanide concentration. The result is similar to that of [56]. They found that ANN was able to predict the concentration of surface runoff water at varying depths and time as depicted by low root mean square error value. A Similar result was obtained in the works of [54,62]. Another similar result was found in the research work of [53]. They normalized there datasets before training, and their model efficiency was enhanced as evident in a high correlation coefficient of over 0.97. Li *et al.* [57] also applied data normalization in their ANN simulation. Their developed ANN model was able to estimate nitrate concentration in the soil as shown by the value of coefficient of determination ($r^2 = 0.83$). Olawoyin [51] was also able to use ANN model to predict the concentration of polycyclic aromatic hydrocarbons (PAHs) as evident in ($R^2 = 0.9994$). Monjardin *et al.* [50] successfully predicted the concentration of Manganese (Mn) in soil and surface water. They employed the mean absolute percentage error (MAPE) and the root mean square error (RMSE) to assess the ANN model efficiency. For the concentration of Mn in the soil they had MAPE and RMSE values of 2.01% and 23.98% respectively while that of surface water for > 1 mg/l of Mn had a better performance (MAPE = 4.61%, and RMSE = 0.17%). They applied 14 input parameters in the training process, and based on correlation analysis the input parameters were further reduced. Based on their results, they concluded that the ANN model will still sufficiently predict Mn concentration even when 4 to 5 input parameters were removed. Ghazi [49] successfully estimated the concentration of heavy metals (cadmium, copper, zinc, nickel, and lead) using ANN. He found the R value to be 0.98763. The results of [63] showed that ANN was able to predict cadmium and lead than ANFIS and MLR with higher R^2 values of 0.83 and 0.86 and low RMSE values of 1.47 and 0.23 respectively. Kim and Gilley [64] also used ANN model to predict nitrate concentration with an R^2 value of 0.97. Hattab *et al.* [52] effectively applied ANN model to predict the concentration of Chromium in a phytoremediated contaminated soil. They had the R^2 value almost to be 0.999 for all the soil amendments. Rohman *et al.* [65] predicted well the nitrate concentration in soil using ANN model as depicted in the R^2 value of 0.973 and 0.970 for the training and validation datasets respectively.

Table 6 Summary of ANN model performance for dry season

Samples		**Performance metrics**			
		MSE	RMSE	R	R^2
Training	63	0.000273332	0.016532755	0.997713	0.995431
Validation	14	0.000241532	0.015541300	0.998920	0.997841
Testing	14	0.000548220	0.023414098	0.997111	0.994230

Table 7 Summary of ANN model performance for wet season

Samples		**Performance metrics**			
		MSE	RMSE	R	R^2
Training	63	0.0250231	0.158186915	0.997205	0.994418
Validation	14	0.0300722	0.173413379	0.888096	0.788715
Testing	14	0.0431356	0.207691117	0.882642	0.779057

The scatter plots of the predicted concentration (output) to that of the actual concentration (target) for the training, validation, testing, and all the datasets for the dry and wet seasons are depicted by Figure 8 and Figure 9 respectively. The predicted model results are in agreement with the experimental values for the training, testing and validation sets as seen in their correlation coefficients (R). The reason for this assertion is that the closer the correlation coefficient is to 1, the better the model.

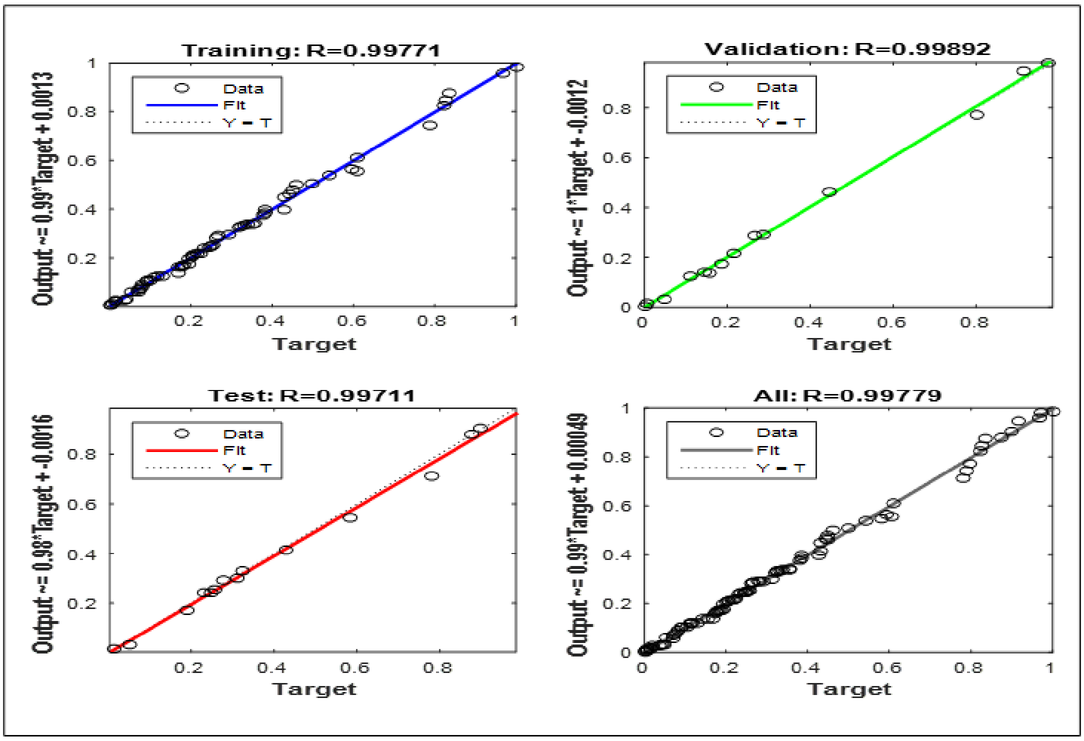

Figure 8 Scatter plots of the developed ANN model for dry season

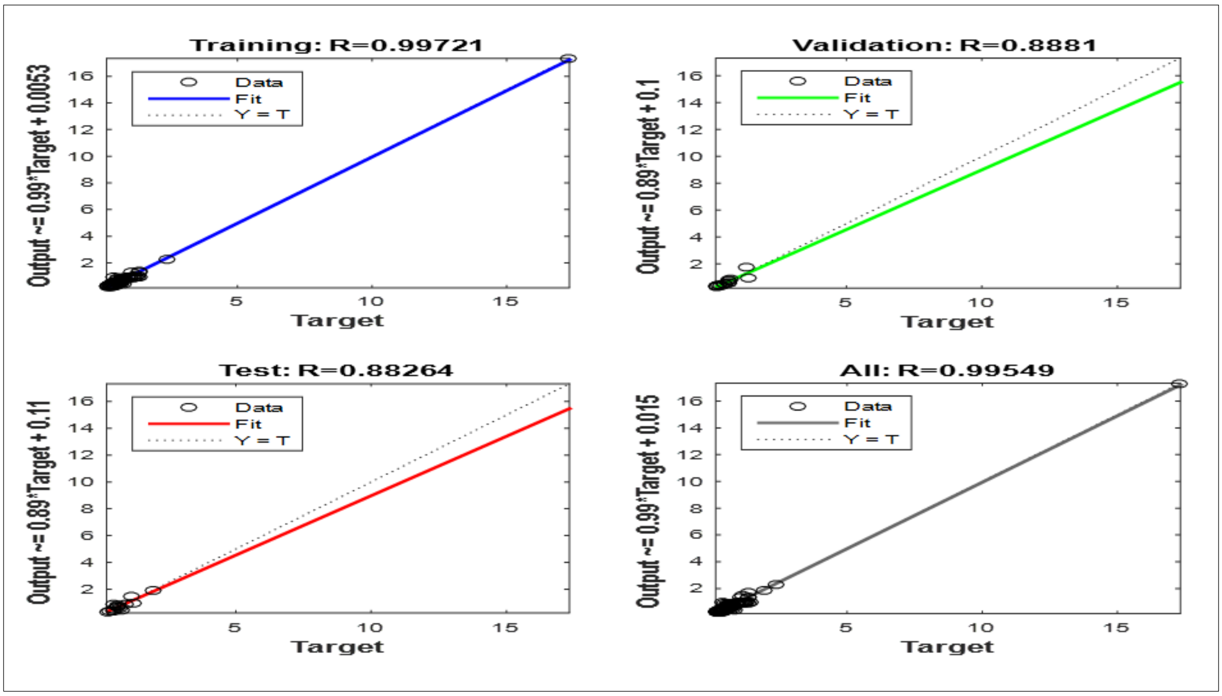

Figure 9 Scatter plots of the developed ANN model for wet season

4. Conclusions

In this study, ANN was used to predict the concentration of cyanide for both dry and wet season. Three input parameters consisting of (depth, time, and measured initial concentration) were used to obtain one output parameter (predicted concentration). The dry season used two neurons in the hidden layer while the wet season used three neurons in the hidden layer to give the best ANN model that predicted the concentration of cyanide in the soil. A total of 91 samples were used for each season and was split into 63 samples for training, 15 samples for validation, and 15 samples for testing.

The performance of the ANN model was evaluated using metrics such as MSE, RMSE, R, and R^2. The results showed that ANN model was able to predict the concentration of cyanide for both seasons as evident in their MSE and RMSE values close to zero and the R^2 value close to unity. However, the data set for dry season had better ANN predictability than that of the wet season as shown by the R^2 values for the training, validation and testing of the dry season to be 0.9954, 0.9978, and 0.9942, while the wet season is 0.9944, 0.7887 and 0.7793 respectively.

Thus, we can conclude that using the data sets of (depth, time, and initial concentration), the concentration of cyanide can effectively be predicted using ANN.

Compliance with ethical standards

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Disclosure of conflict of interest

No conflict of interest to be disclosed.

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