

Application of Particle Swarm Optimisation to achieve simultaneous nitrification and denitrification removal in the aerobic biological treatment process

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Research Article

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Posted Date: August 3rd, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10406672/v1>

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Additional Declarations: No competing interests reported.

Application of Particle Swarm Optimisation to achieve simultaneous nitrification and denitrification removal in the aerobic biological treatment process

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Abstract

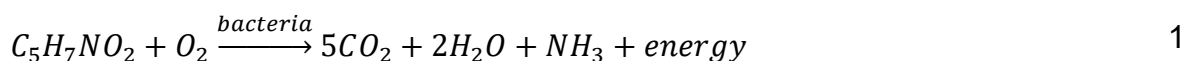
One of the responsibilities of the aerobic biological treatment process is to perform the nitrification process. The nitrification process occurs in two stages: ammonia is oxidised to nitrite by ammonia-oxidising bacteria (AOB), and nitrite is subsequently oxidised to nitrate by nitrite-oxidising bacteria (NOB). In this process, nitrate becomes the residue and if significant quantities are discharged into the environment, high health risks such as digestive tract cancers will be traceable hence, a separate denitrification process is traditionally applied. This study aimed to apply optimisation techniques to achieve the simultaneous nitrification and denitrification process by applying Particle Swarm Optimisation (PSO) algorithm. The input variables applied were: biomass concentration, temperature, ammonia, aeration period, airflow rate, DO, and COD. The PSO algorithm achieved satisfactory results, with a global optimal of 0.5744 mg/L in the following operating conditions: aeration period (1.514 hours), airflow rate (2.6911L/min), DO (5.5768 mg/L), and temperature (30.5270°C). The COD and ammonia concentration outputs were 35.8187 mg/L and 2.9126 mg/L respectively. Temperature (54.2%) and aeration period (22.5%) were the principal drivers of nitrate concentration accumulation in the aeration unit.

Keywords: Nitrification, Denitrification, Optimisation, Biological treatment process, Wastewater treatment plant

1. Introduction

Wastewater treatment plants (WWTPs) have existed for centuries and their main purpose is to purify wastewater that results from residential and industrial areas (Maktabifard et al. 2023). Wastewater treatment takes place in several processes: physical, biological, and chemical (Rashid et al. 2021). The physical processes focus on the removal of large objects and grit to prevent damage to pumps and equipment downstream (Raouf et al. 2019). The biological treatment process is the heart of the WWTP and facilitates the removal of organic and inorganic matter from wastewater (Khalidi-Idrissi et al. 2023). The chemical treatment process concludes the treatment by disinfecting the effluent wastewater, which ensures bacteria are not released into the environment (Crini and Lichtfouse 2019).

The aerobic biological treatment process can be contended as the most important treatment process because it converts organic and oxidises inorganic matter into simple end products. Failure to do so can cause dissolved oxygen (DO) concentration depletion, and uncontrolled eutrophication. Removal of organic matter is quantified either as chemical oxygen demand (COD) or biochemical oxygen demand (BOD), while the removal of inorganic matter is referred to as the nitrification process. The removal of organic and inorganic matter depends on readily available microorganisms in the wastewater. The stoichiometry of aerobic biological organic and inorganic matter removal are shown in Equations 1, 2, and 3.



The nitrification process occurs in two stages. First, ammonia is oxidised to nitrite by ammonia-oxidising bacteria (AOB). Second, nitrite is oxidised to nitrate by nitrite-oxidising bacteria (NOB) (Mousavi et al. 2017; Ribeiro et al. 2018). Equations 2 and 3 show that, upon reducing ammonia concentration to tolerable levels, nitrate concentration accumulates in the aeration unit. If significant quantities of nitrate concentration are discharged into the environment, high health risks such as digestive tract cancers will be traceable (Grout et al. 2023). This short fall has resulted in the addition of configurations such as denitrification process, which is responsible for the

removal of nitrate to nitrogen gas. WWTPs are designed with either a pre-anoxic or post-anoxic denitrification process configuration, which enables ammonia and nitrate removal from wastewater. This has made it difficult for plant operators/managers to achieve complete removal of both ammonia and nitrate. Therefore, a simultaneous nitrification-denitrification process is required to eliminate the accumulation of nitrate during ammonia removal without having a coupled configuration.

Research has been conducted by different scholars in attempts to mitigate the accumulation of nitrate during the removal of ammonia. (Hariri and Botte 2023) reported the use of Pulse Electrolysis Method for simultaneous ammonia and nitrate removal. Ammonia and nitrate effluent quality results were 5.17 mg/L and 0.074 mg/L respectively. Xu et al. (2021) reported the use of microbial electrolysis cell to achieve nitrification and denitrification processes. Microbial electrolysis cell applications serve as electron donors for autotrophic denitrification, enabling the reduction of nitrate in the biological treatment process. The results showed high nitrogen removal of 695.6 g N/m³/d at microbial electrolysis cell of 0.2 voltage. The only challenge with this method is that accumulation of nitrite in the cathode chamber cannot be avoided.

Kondaveeti et al. (2022) utilised a microbial electrolysis cell as a single dual-chamber. The authors achieved total nitrogen removal of 96.8%, 94.11%, and 87.05% at 1.5 V, 1 V, and 0.7 V, respectively. The results were comparable to the results obtained by (Xu et al. 2021), expect that the highest voltage used was 1.5 V. Again, this method has a disadvantage of the electric power required, which increases the overall energy consumption in the WWTP. Tian et al. (2024) reported the use of a combined partial denitrification-anaerobic ammonium oxidation-bioelectrochemical system. With the microbial community changes and improved nitrogen metabolism-related genes, a 90% nitrogen removal efficiency without nitrate accumulation. Ye et al. (2019) reported the use of Activated Carbon/Zinc Ferrite Hybrid Catalyst under UV-Visible Irradiation. The Activated Carbon/Zinc Ferrite Hybrid Catalyst functioned as a photocatalyst. The results showed a 90.2%, 92%, and 90% removal for total nitrogen, nitrite, and ammonia. The final product released in the reaction was nitrogen gas.

Pang et al. (2023) reported the use of hydrogen-based partial denitrification paired with anammox in a membrane biofilm reactor. The authors used anammox which enabled an effective removal of nitrogen. Furthermore, hydrogen-derived membrane

biofilm reactors where used as a replacement for the traditional partial denitrification, resulting in nitrate reduction. simultaneous removal of ammonia and nitrate is possible. The results showed an increase from 57.1% to 93.7% total nitrogen removal. Fan et al. (2021) reported the simultaneous removal of advanced stacked assembly biological filter. The authors assembled biological filters with solid polymeric ferric sulphate and alternating anaerobic and aerobic. This configuration resulted in the effective removal of ammonia (87%), total nitrogen (83.4%), COD (91%), and total phosphorus (80%).

The literature review detailed above has shown significant contribution to address this problem. However, the methods proposed in the literature are not cost-effective and cannot be simply integrated into an existing conventional WWTP. The disadvantage of using Pulse Electrolysis and microbial electrolysis cell is that electric power is required, which increases the overall energy consumption in the WWTP. The use different configuration does not assist the existing WWTPs, since they have already be designed and constructed to operate in a certain way. A different configuration will require a complete overhaul of the WWTP. This study proposes an optimisation technique that will use the current operating parameters in the biological treatment process.

Optimisation is a technique used for maximising or minimising real-life problems to attain enhanced functional settings of a system (Engelbrecht 2007). In WWTPs, optimisation processes have been applied to enhance the performance, minimise energy consumption, obtain bioreactors process control parameters, improve grit removal and screening processes, improve the disinfection process, reduce WWTP construction costs, maximise wastewater reuse, and increase efficiency in sedimentation tanks (Geem et al. 2018; Denysiuk et al. 2018; Panepinto et al. 2020; Borzooei et al. 2019; Mirzaie et al. 2021; Rafati et al. 2020; Muloiwa and Ndambuki 2026). In this study, optimisation technique will be used to minimise nitrate accumulation, which will enable the simultaneous nitrification and denitrification process in the biological aeration unit.

2. Methods and materials

2.1 Wastewater collection and disposal

Wastewater was collected from the Daspoort wastewater treatment plant, in South Africa. The Standard Methods for the Examination of Water and Wastewater Manual

was applied during wastewater handling and equipment use. The second aeration chamber was used for this research. Wastewater was collected in the morning at 09:00 am, and in the afternoon between 14:30 and 15:00, with the aim of collecting wastewater utilised and discharged by the city in the early hours and midday, respectively. Wastewater was collected over 54 days using a two-litre bottle and 25-litre container for activated sludge raw wastewater respectively. Both wastewater and activated sludge were used within two hours of collection to avoid biological activity. Wastewater was disposed of in the laboratory ablution facilities after completing the aeration process.

2.2 Aeration and Data Collection

Figure 1 shows the aeration chamber set up, where the aeration process was performed. The aeration airflow rate was kept at five litres per minute (L/min) utilising an air diffuser and an air blower. The temperature range applied in the research was between 15°C – 35°C, which represents cold and warm weather temperatures. Ice cubes were utilised to regulator the temperature between 15°C and 22°C whereas a thermostat was utilised to regulate the temperature between 22°C and 35°C. A hydraulic retention time of four hours was applied, and wastewater was sampled to measure the wastewater characteristics concentration as follows: initial, second hour, and fourth hour. 324 data points were collected during the aeration process. Wastewater characteristics measured were: nitrate, COD, ammonia, and biomass concentrations. The following methods, detailed in the Standard Methods for the Examination of Water and Wastewater Manual, were applied to measure wastewater characteristics concentration.

- Nitrate – APHA (2012) method 4500
- COD – APHA (2012) method 5220
- Ammonia – APHA (2012) method 4500
- Biomass concentration – Optical density methods and Cell dry density

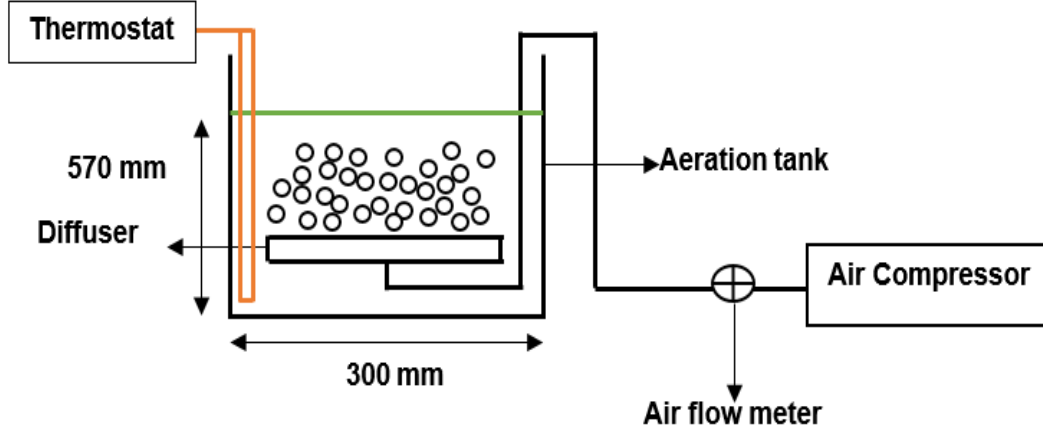


Figure 1: Laboratory biological aeration chamber

2.3 Modelling

A nitrate concentration regression model was developed in MATLAB using the Multilayer Perceptron (MLP) Artificial Neural Network (ANN) algorithm. The general form of the MLP ANN algorithm is defined in Equation 4.

$$Y_i = f\left(\sum_{j=1}^N W_{ij}X_j + bi\right) \quad 4$$

Where W_{ij} and b is the weighting factor, and bias of the i th node, f is the activation function, X is the j th nodal value for the previous layer, and Y is the i th nodal value in the current layer. The following procedure was followed when applying the MLPANN algorithm: Select input variables, data was split into 70% (training), 15% (validation), and 15% (testing), a normalization method was applied to transform data (Equation 5), two hidden layers and nine neurons were applied to produce the MLPANN architecture (Figure 2). The MLPANN algorithm was run using a sigmoid activation function (Equation 6) and a gradient descent backpropagation learning algorithm. The model performance was evaluated using the following metrics: MSE, R^2 , and RMSE defined by Equations 7, 8, and 9, respectively.

$$x(\text{scaled}) = \frac{x - \min_x}{\max_x - \min_x} \quad 5$$

$$f = \frac{1}{1 + e^{-x}} \quad 6$$

$$MSE = \sum_{i=1}^n \frac{(\hat{y}_i - y_i)^2}{N} \quad 7$$

$$R^2 = \frac{1}{m} \sum_{j=1}^m \left(1 - \frac{SSE}{SST} \right) \quad 8$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{N}} \quad 9$$

The input variables utilised for predicting nitrate concentration were: COD concentration, aeration period, ammonia concentration, biomass concentration, airflow rate, DO, and temperature as shown in Figure 2.

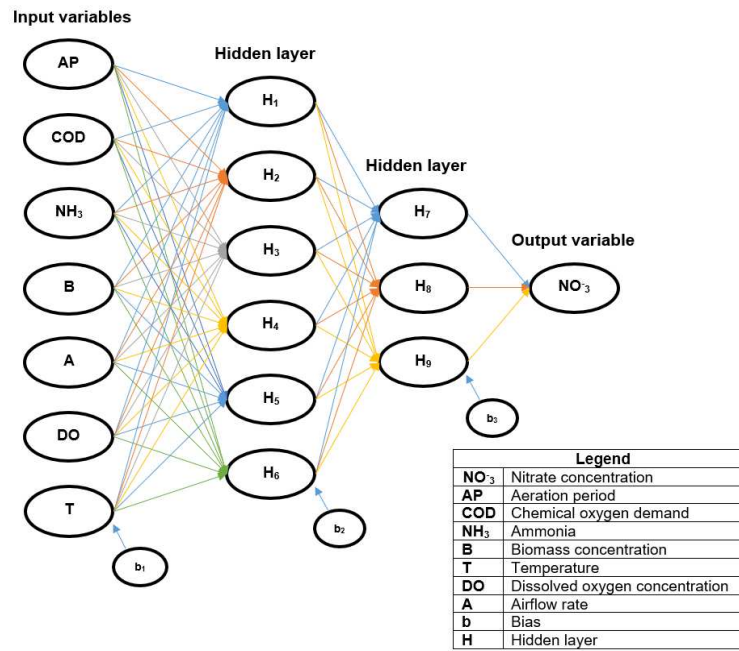


Figure 2: MLP ANN Architecture

2.4 Particle Swarm Optimisation

A nitrate concentration optimisation model was considered as the objective function. The general formula that describes the optimisation of nitrate concentration is defined in Equation 10.

$$\text{Minimize}[Y_i(AP, T, COD, NH_3, B, AR, DO,)] \quad 10$$

Where: Y_i is the nitrate concentration model, COD is the Chemical oxygen demand, AP is the aeration period, NH_3 is the ammonia concentration, AR is the airflow rate, DO is the dissolved oxygen concentration, B is the biomass concentration, and T is the Temperature. The constraints applied in the optimisation process are defined by Equations.

$1 \leq AP \leq 4 \text{ hours}$	11
$30 \leq COD \leq 75 \text{ mg/l}$	12
$1 \leq NH_3 \leq 3 \text{ mg/l}$	13
$0.1 \leq B \leq 6.512 \text{ g/l}$	14
$1 \leq AR \leq 5 \text{ l/min}$	15
$0.5 \leq DO \leq 8 \text{ mg/l}$	16
$15 \leq T \leq 35^\circ\text{C}$	17

The pseudo-code shown in Table 1 was followed to optimise the nitrate concentration model. The velocity and position of each particle in the search space were updated using Equations 18 and 19, respectively.

$$x_{ij}(m+1) = x_{ij}(m) + v_{ij}(m+1) \quad 18$$

$$v_{ij}(m+1) = w \times v_{ij}(m) + c_1 \times r_1 (pbest_{i,j} - x_{i,j}(m)) + c_2 \times r_2 (gbest_j - x_{i,j}(m)) \quad 19$$

Table 1: Particle swarm optimisation PSEUDO CODE

Particle Swarm Optimization (PSO) Algorithm	
1.	Initialize the particles' position (x^i), velocity (v^i), previous best position (p^i), and the number of particles N
2.	While (t < maximum number of iterations (T)) do
3.	For all Particles (i) do
4.	Calculate the fitness function for the current position x_i of the i^{th} particle ($F(x^i)$)
5.	If ($F(x^i) < F(p^i)$) then
6.	$P^i = x^i$ end if
7.	If ($F(x^i) < F(G)$) then
8.	$G = x^i$
9.	End if
10.	Adjust the velocity and positions of all particles according to equations 18 and 19, respectively.
11.	End for
12.	Stop the algorithm if a sufficiently good fitness function is met
13.	End while

2.5 Sensitivity analysis

Sensitivity analysis was conducted on the optimising model (nitrate concentration). A one-factor-at-a-time method was utilised. Each decision variable was individually adjusted by $\pm 10\%$, $\pm 20\%$, and $\pm 50\%$, while the other variables were kept untouched. In addition, decision variables were confirmed for their inverse, direct, minor, or major changes in the optimised nitrate concentration model.

3. Results and discussions

3.1 Laboratory results

Table 2 details the correlation matrix results. Nitrate concentration was positively correlated to aeration period (0.566**), biomass concentration (0.734**), and temperature (0.692**). The positive correlation between aeration period and nitrate concentration shows that during aeration, nitrate accumulates in the aeration unit. This is due to the nitrification process, which occurs in two stages: ammonia is oxidised to nitrite by AOB and nitrite is oxidised to nitrate by NOB. Hence, the link between nitrate and ammonia produced a negative correlation of -0.759**. The positive correlation between biomass concentration and nitrate concentration shows that when microorganisms (AOB and NOB) oxidise ammonia in the presence of DO, ammonia is reduced and nitrate is produced. Temperature increases bacteria growth rate, which accelerates the nitrification process, hence nitrate concentration increases when temperature increases in the aeration tank.

Table 2: Correlation matrix results

	NO ₃ ⁻	AP	COD	NH ₃	B	AR	DO	T(°C)
NO ₃ ⁻	1							
AP	.566**	1						
COD	-.419**	-.860**	1					
NH ₃	-.759**	-.759**	.712**	1				
B	.734**	.603**	-.578**	-.700**	1			
AR	0.013	0.000	0.008	.020*	-.101**	1		
DO	-.473**	.135**	-.250**	.214**	-.222**	.124**	1	
T(°C)	.692**	0,000	.123**	-.392**	.403**	0,000	-.848**	1
**. Correlation is significant at the 0.05 level (2-tailed).								
Temperature (T °C), ammonia (NH ₃), nitrate (NO ₃ ⁻), biomass concentration (B), airflow rate (AR), Dissolved concentration (DO), Aeration period (AP)								

3.2 Modelling

3.2.1. Prediction accuracy

The MLPANN algorithm was able to model the nitrate concentration data in the aeration unit. Figure 3 (A), (B), and (C) show the prediction accuracy between the predicted and observed data. When the data points form the valley and ridge shape, the MLPANN algorithm worked hard to predict the data points. This is due to the

disadvantage of mathematical models, unable to predict peak values. However, in the case of nitrate concentration prediction, an accurate pattern can be observed during the training, validation, and testing datasets as shown in Figure 3 (A), (B), and (C).

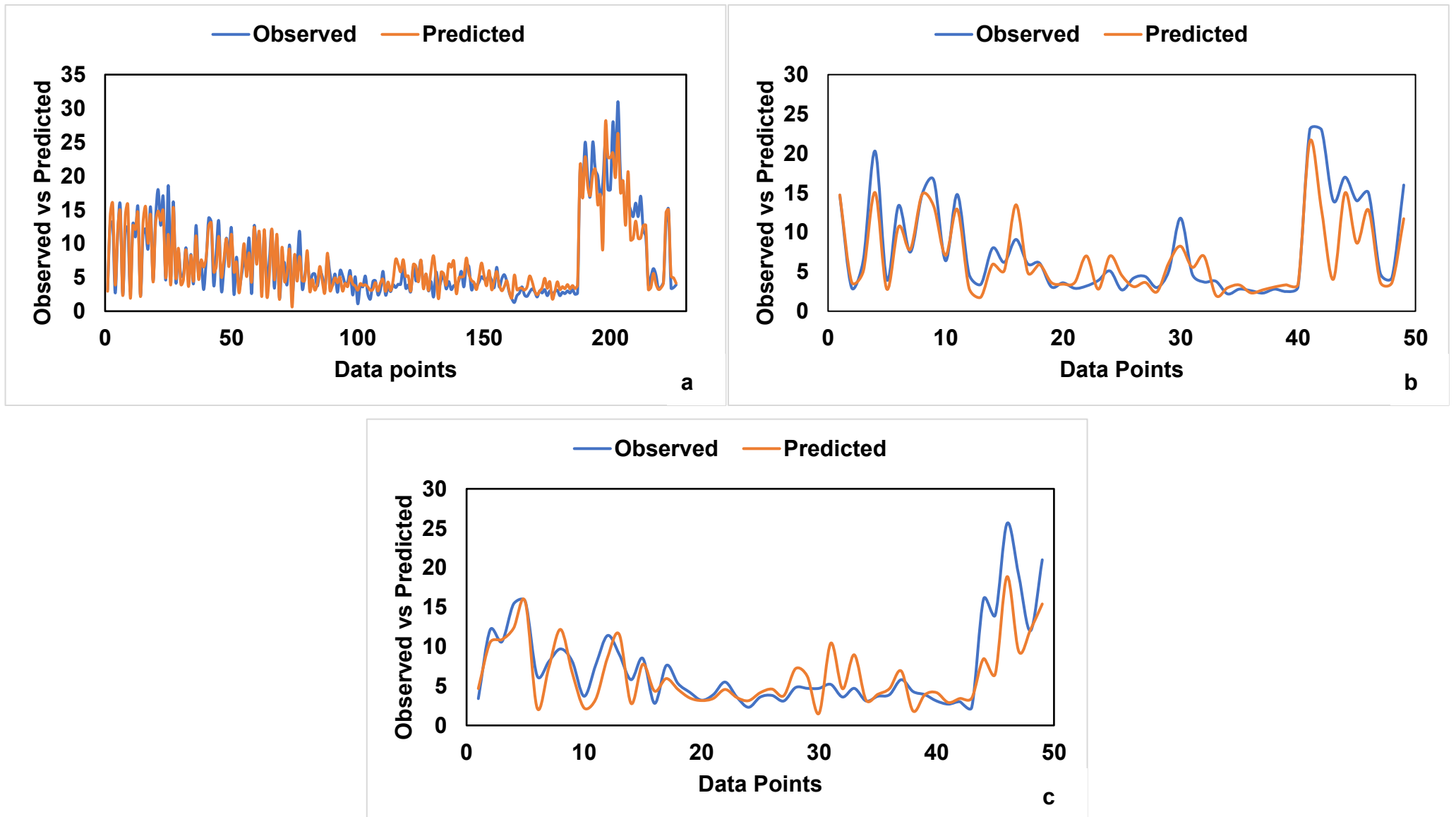


Figure 3: Predicted vs Observed data during the training (a), validation (b), and testing (c) phases

3.2.2. Model performance evaluation

The MLP ANN algorithm performance was satisfactory and produced a MSE of 3.2614 during the validation phase after performing 23 iterations (Epochs). The low MSE value (3.2614) obtained indicates that the data points are closely stacked to the mean, which suggests that limited errors will be observed between each data point and the mean value of the data points. Since the MSE value is close to zero, it provides confidence that the nitrate concentration model will perform at a high level to ensure accurate prediction.

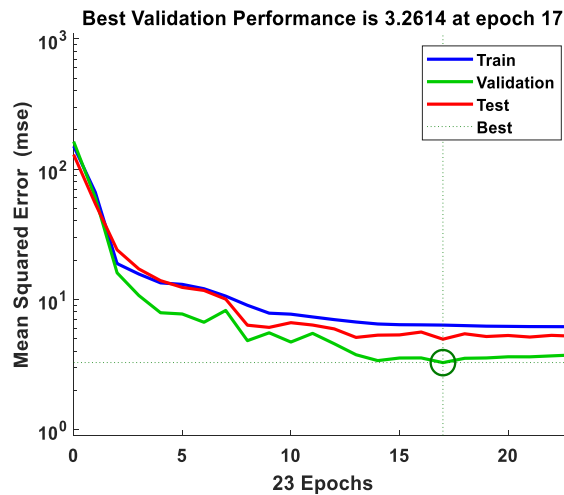


Figure 6: MSE during nitrate concentration prediction

In addition to the confidence provided by the low MSE value, R^2 values throughout training (0.897), validation (0.893), testing (0.946), and combined (0.909) produced satisfactory results as shown in Figure 6 (A), (B), (C), and (D), respectively. This signifies that 94.6% of the output data (nitrate concentration) can be explained by the input data (COD, aeration period, ammonia, biomass, airflow rate, DO, and temperature) during the testing phase of the model. The nitrate concentration model improved from the training phase to the testing phase, which shows the robustness of the MLP ANN algorithm in modelling complex data patterns. Because the R^2 values during all learning phases are close to a value of one (1), it provides confidence that the nitrate concentration model will perform at a high level to ensure accurate prediction, despite notable outliers.

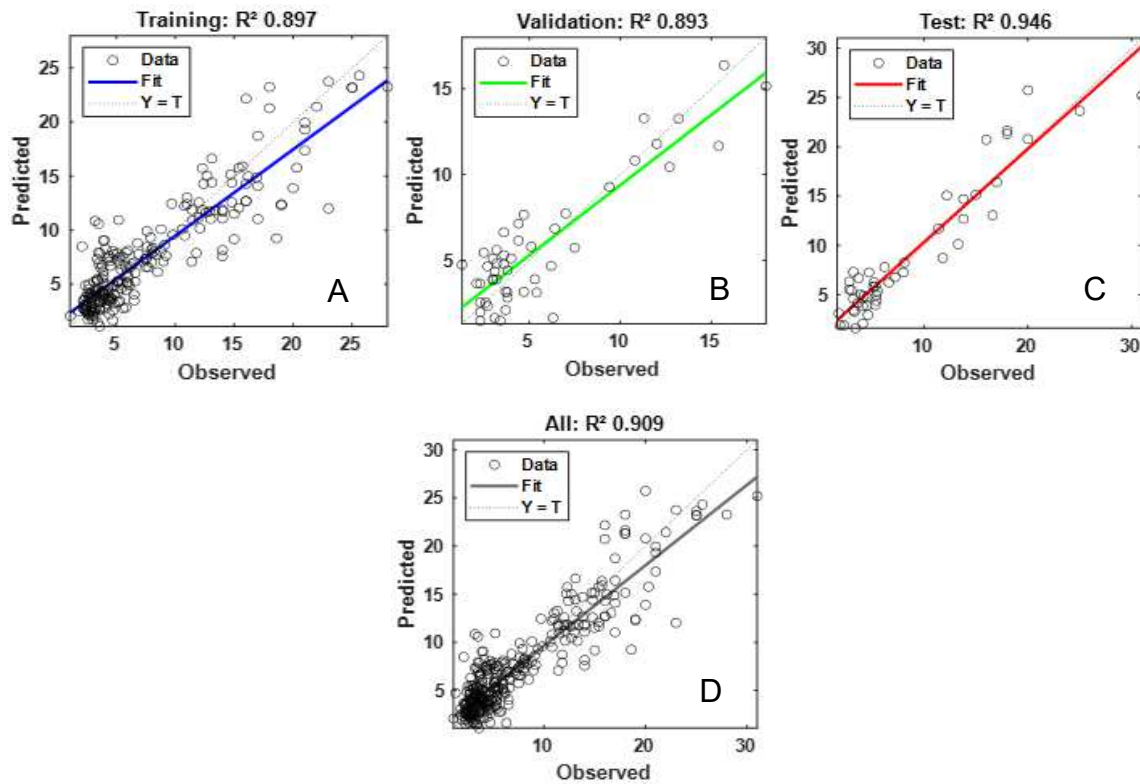


Figure 7: Coefficient of determination during training (A), validation (B), testing (C), and All combined data (D)

RMSE values provided further confidence of the nitrate concentration model. The validation phase produced the lowest RMSE of 1.806 as shown in Figure 7. This suggests that the average difference between MLP ANN nitrate concentration model data and the observed nitrate concentration data is low. This statistical measure provides further confidence that the nitrate concentration model will provide accurate prediction when used to predict nitrate concentration in the aeration unit.

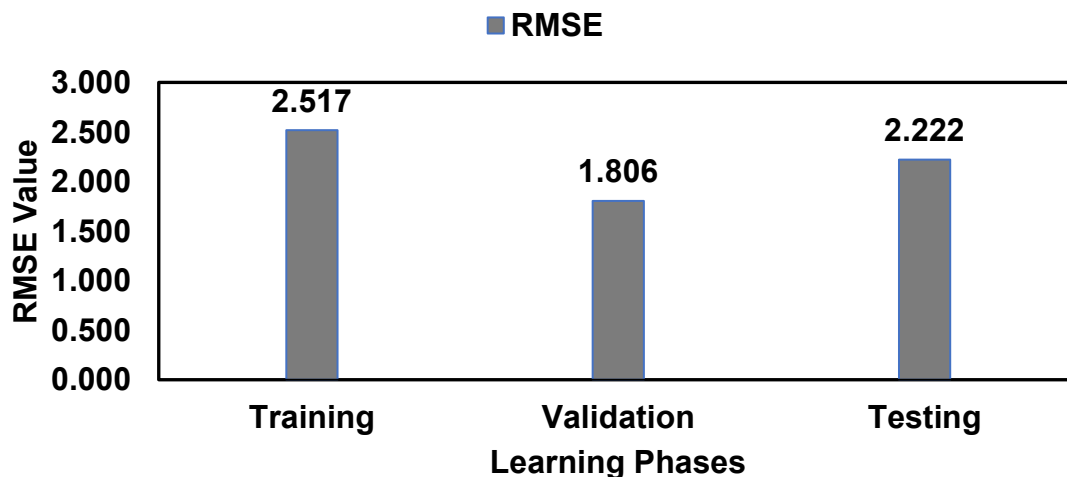


Figure 8: RMSE during nitrate concentration prediction

3.3 Optimisation

Figure 8 presents the relationship between the optimal nitrate concentration and the number of iterations. The PSO algorithm converged after 1000 iterations and produced a global optimum value of 0.5744 mg/L, as shown in Figure 8. The global optimum value (0.5744 mg/L) was within the acceptable discharge standards (1.5 – 3 mg/L) set out by the Department of Water and Sanitation. This indicates that simultaneous nitrification and denitrification are possible in the aeration process.

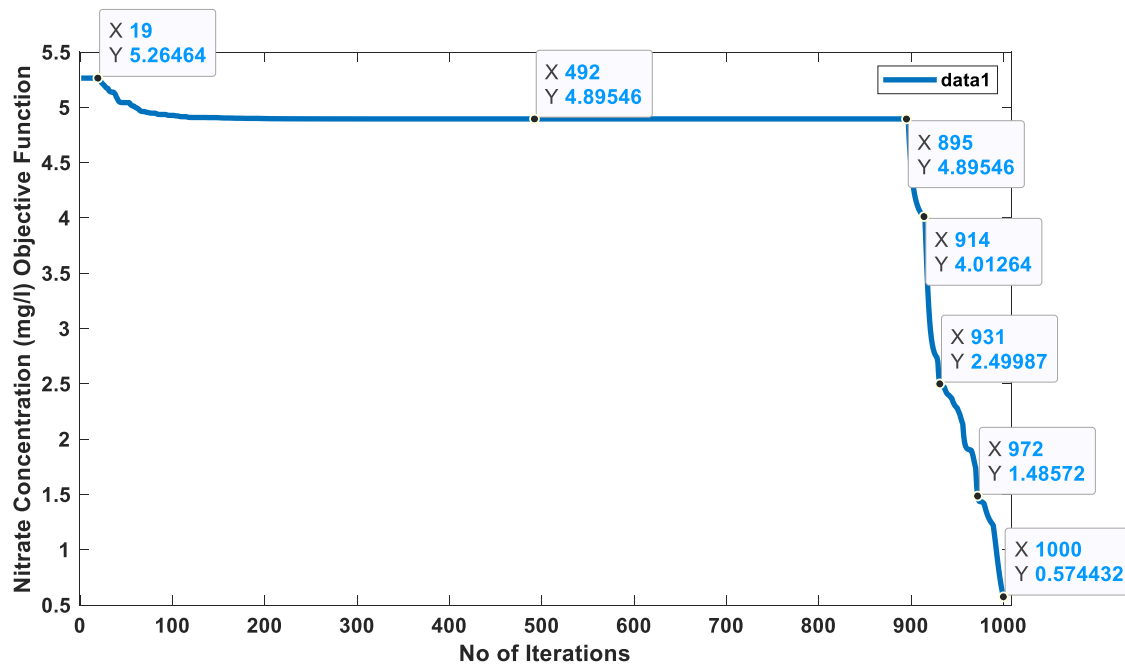


Figure 9: Optimum fitness function value

Table 3 presents the input variables' operating conditions that enabled nitrate concentration to be suppressed in the aeration unit. When the aeration unit is operated for 1.4157 hours, at an airflow rate of 2.6911 L/min, a temperature of 30.5270°C, and a DO concentration of 5.5768 mg/L, the effluent COD concentration, ammonia concentration, and nitrate concentration will be 35.8187 mg/L, 2.9126 mg/L, and 0.5744 mg/L, respectively. Operating the biological aeration unit at a higher temperature (30.5270°C), influenced rapid COD and ammonia removal in a short hydraulic retention time (1.4157 hours). This provides confidence that the nitrification and denitrification processes can take place simultaneously in the aeration unit. The

Table 3: Input variables operating conditions

No	Input variables	Optimised results
1	AP (hours)	1.4157
2	COD (mg/L)	35.8187
3	Ammonia (mg/L)	2.9126
4	Biomass (g/L)	1.9343
5	AR (L/min)	2.6911
6	DO (mg/L)	5.5768
7	T (°C)	30.5270

Figure 8 and Table 4 shows the observed verses optimised data points. 80 observed data points were applied in the optimised nitrate concentration model as shown in Figure 8 and Table 4. The sum of the observed (368.829 mg/l) and optimised (152.557 mg/l) data points showed a 58.6% difference, which indicates that the optimised data points were minimised. Similarly, the average of the observed and optimised data points showed a difference of 58.7% difference, which justifies that the nitrate concentration was minimised. In addition, the ANOVA test results show that the F – critical (3.9) value was lower than the F – statistic (348.535) value, which confirms that there was a significant difference between the observed and optimised nitrate concentration data. The P-value was lower than the significance level of 0.05, which justifies that the significant difference between the observed and optimised nitrate concentration data.

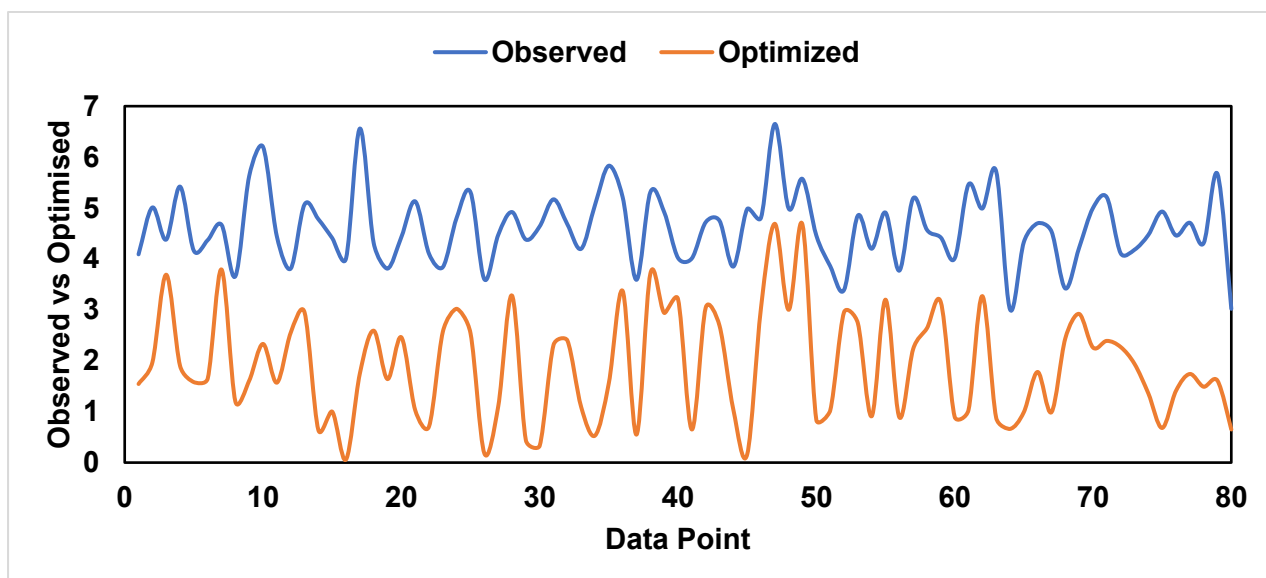


Figure 8: Observed vs Optimised data points

Table 4: Descriptive statistic summary and ANOVA test on observed verses optimised data

SUMMARY				
Groups	Count	Sum	Average	Variance
Observed	80	368.829	4.61036	0.51226
Optimised	80	152.557	1.90696	1.16524
ANOVA				
F – Statistic	P-value	F – Critical		
348.535961	8.2E-42	3.90099		

3.4 Sensitivity analysis

Figure 9 and Figure 10 presents the sensitivity analysis of the optimised nitrate concentration model and the relationship between input variables and the nitrate concentration optimised model output respectively. Two out of the seven input variables showed to be the principal drivers of the nitrate concentration in the aeration unit. Temperature (54.2%) was the highest contributor followed by aeration period (22.5%). This means that the two variables (Temperature and aeration period) can be used to predict nitrate concentration in the biological aeration unit. Five variables: aeration period, biomass concentration, airflow rate, DO, and temperature increased with an increase in nitrate concentration as shown in Figure 10 (A), (D), (E), (F), and (G) respectively. The most notable was aeration period which produced the highest linear regression slope line of 4.2694 hour. Nitrate concentration increased with a decrease in COD and ammonia concentration at a rate of 0.0019 mg/l and 0.5268 mg/l respectively.

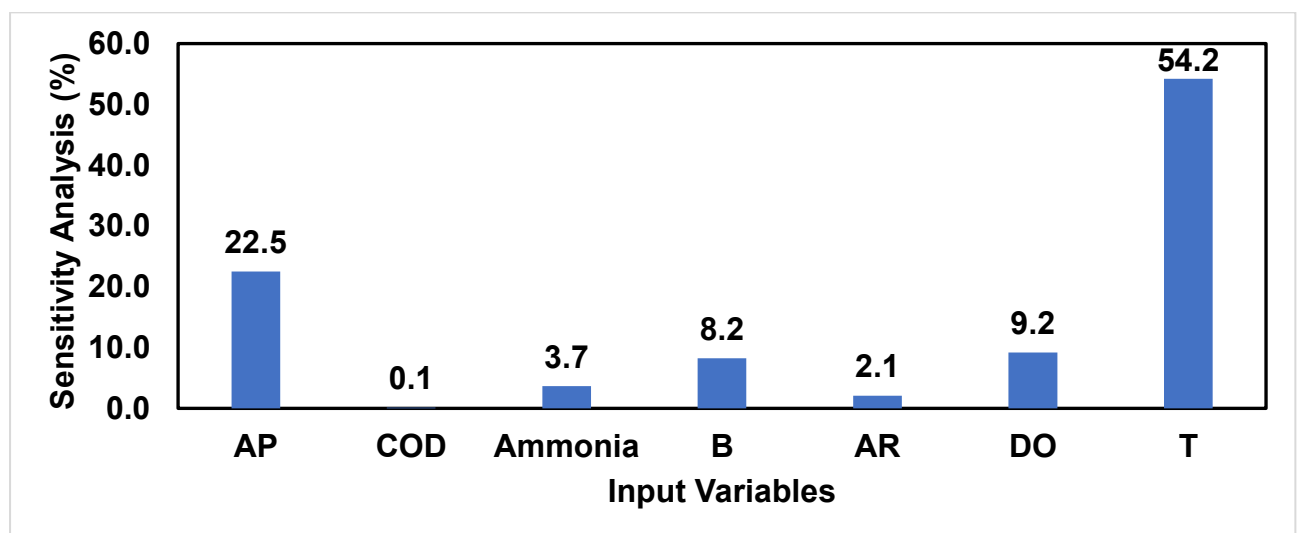


Figure 9: Sensitivity analysis of the optimised nitrate concentration model

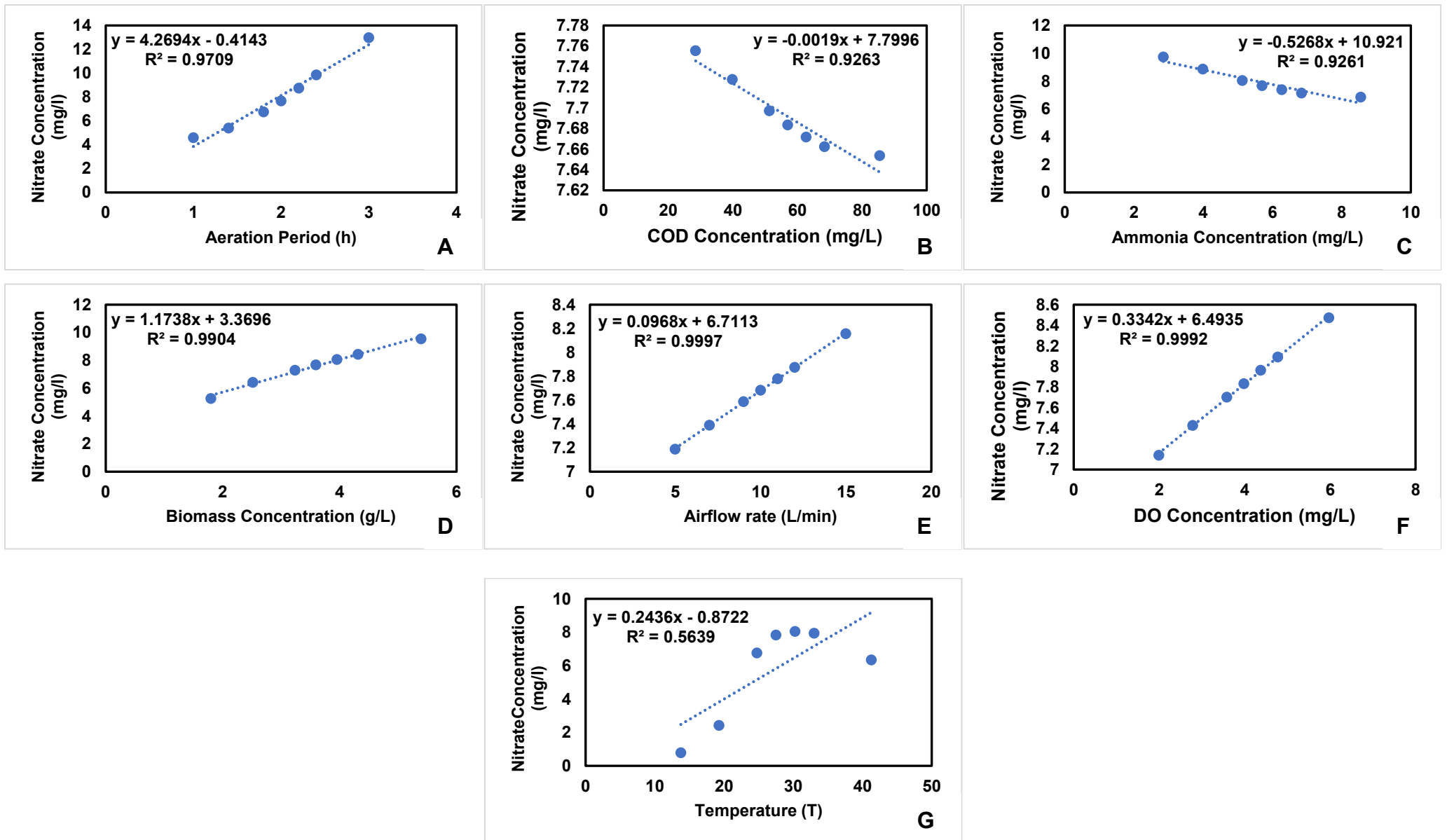


Figure 10: Relationship between input variables and the nitrate concentration optimised model output

4. Conclusions

The aim of the study was to optimise nitrate accumulation in the aeration unit such that simultaneous nitrification and denitrification processes can be achieved. Nitrate concentration was modelled and optimised using MLP ANN algorithm and PSO algorithm. The following input variables were utilised: aeration period, COD, ammonia, biomass concentration, airflow rate, DO, and temperature. The PSO algorithm achieved satisfactory results and produced a global optimum solution of 0.5744 mg/l in the following operating conditions: aeration period (1.514 hours), airflow rate (2.6911 l/min), DO (5.5768 mg/l), and temperature (30.5270°C). The COD and ammonia concentration output were 35.8187 mg/l and 2.9126 mg/l respectively. Temperature (54.2%) and aeration period (22.5%) were the biggest drivers of nitrate concentration in the aeration unit. Simultaneous nitrification and denitrification can be achieved using optimisation techniques in the aeration unit.

5. Funding Declaration

No funding was obtained for this research study.

6. Declarations

Ethics, Consent to Participate, and Consent to Publish declarations: not applicable.

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