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Evaluation of Artificial Neural Networks for Electrical Conductivity-based and Flow Rate-based Prediction of the Nitrate Nitrogen Concentration in the U-Tapao Canal, Hat Yai, Thailand

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Abstract

The aim of this study was to identify suitable artificial neural network (ANN) models for the EC-based and flow rate-based prediction of the nitrate nitrogen (NO_3-N) concentration in the U-Tapao canal, located in the southern part of Thailand. Two types of four layer ANNs of the feed-forward back propagation (FFBP) and cascade-forward back propagation (CFBP) types were evaluated for this prediction. The selected inputs of the ANNs were EC and flow rate, which were collected daily from December 2014 to March 2015. Overall, the study found that the four layer FFBP with 2 neurons in the input layer, 20 neurons in the first hidden layer, 30 neurons in the second hidden layer, and a single neuron in the output layer with a tan-sigmoid transfer function was the optimal model. The FFBP model produced slightly more accurate results than the CFBP model. Linear regression analysis was used to predict NO_3-N, which was compared with the results of the ANNs and the performance of the ANNs was better than that of the linear regression analysis. Therefore, the ANN approach proved to be suitable as an alternative to laboratory-based analysis for the prediction of NO_3-N values in the U-Tapao canal.

Keywords: nitrate nitrogen concentration prediction; artificial neural network (ANN); U-Tapao canal; model

1. Introduction

The U-Tapao canal sub-basin located in Songkhla province, southern Thailand is a sub-basin of the Songkhla Lake basin. In this sub-basin, the U-Tapao canal is an important raw water resource, which supplies water to Hat Yai district, Thailand. The canal is surrounded by agricultural land, factories, communities and urban areas (Office of Natural Resources and Environmental Policy and Planning, 2011). Thus, it receives effluent from wastewater treatment systems and wastewater which are untreated point and non-point sources of effluent. A large amount of nitrogen leaches into the U-Tapao canal, and is then transported to Songkhla Lake. This has caused ecological impacts such as eutrophication and oxygen deficiency.

In order to monitor and maintain suitable water quality, monitoring on essential water quality is necessary. Water sampling and analysis have to be performed at regular intervals for water quality monitoring. The water quality parameters of interest require laboratory-based measurement in order to obtain accurate values from water samples. The necessity of frequently sampling water and analyzing it with laboratory-based measurements can be time-consuming and expensive (Pongpetch *et al*., 2015). Therefore, water quality models can be used as a low cost alternative tool for water monitoring, and can supplement laboratory analysis.

The relationship between water quality parameters is used to identify a suite of easy-to-measure indices for evaluating the parameters of interest, for example, total solids (TS) and electrical conductivity (EC) are employed as surrogate parameters for total phosphorus (TP) (Miguntanna, 2009; Miguntanna *et al*., 2010), and chloride (Cl^-) (Welagedara *et al*., 2014), respectively, and total nitrogen concentration can also be estimated from EC (Yamazaki *et al*., 2014). EC is the measurement of the ability of water to conduct an electric current, it approximates the overall concentration of total dissolved inorganic ions (Talling, 2009). Nitrate ions are one of the major ion constituents in surface waters (Clarke, 1924; Nhantumbo *et al*., 2016) which directly affect EC values. Therefore, it is possible to find a correlation between EC and nitrogen concentrations. EC can be used to estimate the nitrate concentrations by developing a linear regression equation (Gali *et al*., 2012; Joarder *et al*., 2008).

Hanslík *et al*. (2016), Jarvie *et al*. (2003), Mosley (2015), and van Vliet and Zwolsman (2008) demonstrated the existence of relationship between water quality and flow rate and in particular, that nitrate concentrations were lower during the low flow rate periods. Lower concentrations of nitrate may be explained by drought conditions (Hanslík *et al*., 2016; van Vliet and Zwolsman, 2008), resulting in a reduced supply from soil leaching and overland flows (van Vliet and Zwolsman, 2008), and increased denitrification (Mosley, 2015). In contrast, in some areas there is a little evidence of a negative relationship between nitrate concentrations and flow, and nitrate concentrations may be caused by point sources of nutrients (industrial, domestic, agricultural wastewater discharges) (Jarvie *et al*., 2003; Mosley, 2015) and lower levels of dilution (Hanslík *et al*., 2016).

The development of useful water quality models poses specific problems, mainly caused by the complicated non-linear characteristics of water quality parameters. In practice, the essential data may be scarce and inaccurate, during some periods. Therefore, traditional mathematical and statistical-based water quality models are difficult and not practicable (Wu *et al*., 2000; Singh *et al*., 2009). However, artificial neural networks (ANNs) can be used to overcome this problem. An ANN model is a computation model based on the human brain. ANNs are very powerful computational techniques for the non-linear complex modeling of relationships between variables (Ranković *et al*., 2010; Singh *et al*., 2009). In recent years, ANNs have been used increasingly for the prediction and forecasting of water quality variables (Maier *et al*., 2010) (e.g. dissolved oxygen (DO) (Sahoo *et al*., 2006; Zou *et al*., 2007), salinity (Bowden *et al*., 2005; Kingston *et al*., 2005), chlorophyll-a (Lu *et al*., 2016)).

In this study, EC and flow rate were selected as the input data parameters. Two types of ANNs, the feed-forward back propagation (FFBP), and cascade-forward back propagation (CFBP) were used to predict NO_3-N values in the U-Tapao canal. Finally, the ANN model results were compared with the results from the linear regression analysis.

2. Materials and Methods

2.1 Study area

The U-Tapao canal sub-basin is the biggest sub-basin in the Songkhla Lake basin, with a drainage area of 2410 km^2. It is a mixed-use basin and a summary of land use in the U-Tapao canal sub-basin is shown in Fig. 1. In this sub-basin, the U-Tapao canal is the most important canal, which flows approximately 175 km to the lower part of Songkhla Lake (Sutiwipakorn and Ratanachai, 2005). Base on GIS data, there are about 300 factories located within U-Tapao canal sub-basin (Chuvanich *et al*., 2017). The majority of land use in this sub-basin is Para rubber plantations, which account for 65 percent of the land use.

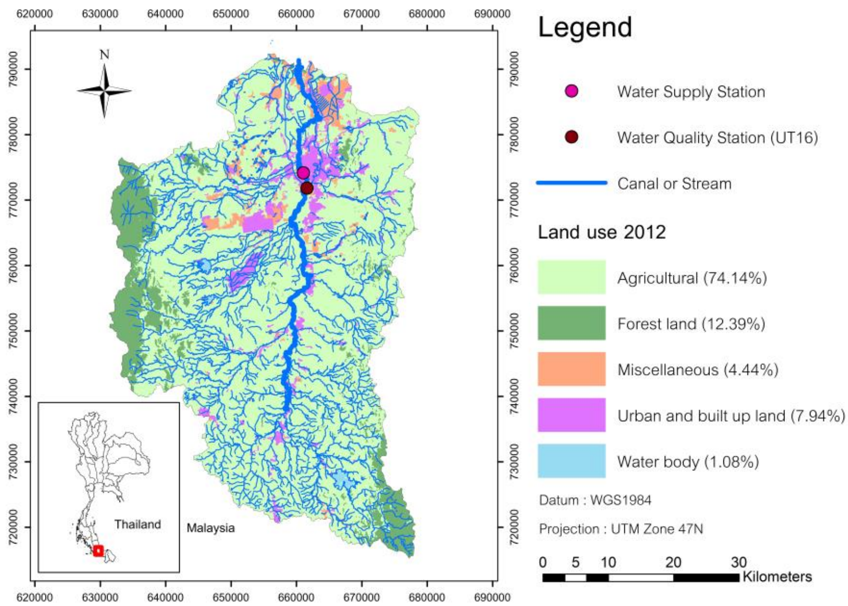

Figure 1. Land use in the U-Tapao sub-basin
(Source: GEO-Informatics Research Center for Natural Resource and Environment**,** Prince of Songkla University)

Table 1. Basic statistics of measured water quality variables and flow rates in U-Tapao canal (Number of samples = 96 datasets)

Variable	Unit	Min	Max	Mean	SD	CV%
NO_3-N	mg/L	0.00	6.60	2.36	1.46	61.66
pH		5.51	6.99	6.47	0.25	3.94
Turbidity	NTU	13.10	512.00	53.18	79.97	150.38
DO	mg/L	2.90	9.00	4.91	0.95	19.33
NH_3-N	mg/L	0.10	2.00	0.53	0.31	59.27
EC	uS/cm	49.90	337.00	172.05	72.05	41.88
Flow rate	(m^3/s)	3.62	725.60	82.71	173.80	210.14

SD= Standard Deviation; CV= Coefficient of Variation

2.2 Input variables and data processing

Water quality data was provided by Hat Yai Water Works Supply, Songkhla, Thailand. The daily values of six water quality parameters (EC, pH, turbidity, DO, ammonia-nitrogen (NH_3-N), and NO_3-N) were measured between December 2014 and March 2015 (96 samples). NO_3-N and NH_3-N values require a laboratory-based measurement, and these were obtained from water samples taken at the UT16 station, approximately 3.2 km from the Hat Yai water supply station. The position of the UT16 and Hat Yai water supply stations are shown in Fig. 1. The flow rates were provided by Regional Irrigation office 16, and the Southern Natural Disaster Research Center. Basic statistics of six water quality parameters and the flow rate are presented in Table 1.

The relationships between the six water quality parameters and the flow rates at the sampling site (UT16) were analyzed using Microsoft Excel correlation analysis. Evans (1996) suggested for the absolute value of correlation, the correlation shows a very strong positive correlation (*r=0.87*) between EC and NO_3-N, while the flow rate and NO_3-N produced the largest negative relationship (*r=-0.59*) and moderate positive correlation, as shown in Table 2. Likewise, EC and NO_3-N showed a positive relationship which supports the hypothesis that when EC increases, NO_3-N will increase, as can be observed in Fig. 2. On the other hand, there was the negative relationship between flow rate and NO_3-N which means that when the flow rate is very high, the NO_3-N will be at a very low concentration, as shown in Fig. 2. Therefore, EC and flow rate were selected for the prediction of NO_3-N level at the UT16 station.

Table 2. Correlation coefficient (*r*) between seven water quality parameters in the U-Tapao canal

Water Quality Variables	NO_3-N (mg/L)	pH	Turbidity (NTU)	DO (mg/L)	NH_3-N (mg/L)	EC (uS/cm)	Q (m^3/s)
NO_3-N (mg/L)	1						
pH	0.19	1					
Turbidity (NTU)	-0.53	-0.05	1				
DO (mg/L)	0.18	0.16	-0.06	1			
NH_3-N (mg/L)	0.27	-0.09	-0.1	-0.13	1		
EC (uS/cm)	0.87	0.25	-0.55	0.16	0.37	1	
Flow rate (m^3/s)	-0.59	-0.12	0.74	-0.03	-0.24	-0.6	1

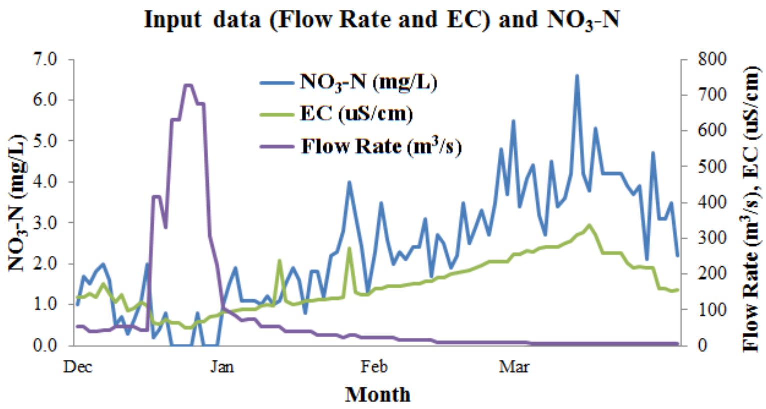

Figure 2. The input data (flow rate and EC) and NO_3-N

2.3 ANN modeling

FFBP (Goyal and Goyal, 2011; Svozil *et al.*, 1997) and CFBP (Goyal and Goyal, 2011; Elbisy *et al.*, 2014) models were constructed for the prediction of the level of NO_3-N. All the ANN models were trained using the Levenberg-Marquardt algorithm (LMA), with two input variables, as shown in Fig. 3. Generic FFBP and CFBP architectures are shown in Figs. 4 and 5, respectively.

The transfer functions of the output and hidden layers were designed in two structures. In the first structure, the non-linear transfer functions, tan-sigmoid and log-sigmoid were used in the output and the first hidden layers, respectively and the linear transfer function, purelin was used in the second hidden layer. In the second structure, log-sigmoid and purelin were used in the output and the first hidden layers, while tan-sigmoid was used in the second hidden layer.

The datasets of EC, flow rates and NO_3-N between December 2014 and March 2015 were divided by the five-fold cross-validation method with the dataset being divided into five subsets. Each time, four subsets were used to train the model and one subset was used to test the model. Each model was run five times. The training and testing dataset were 233 and 96 samples, respectively. The validation dataset, was made of 8 samples collected between April and June 2015, and was a new dataset that had never been used during the training and testing processes. All the ANN models were run on MATLAB software (MathWorks, Inc., Natwick, MA).

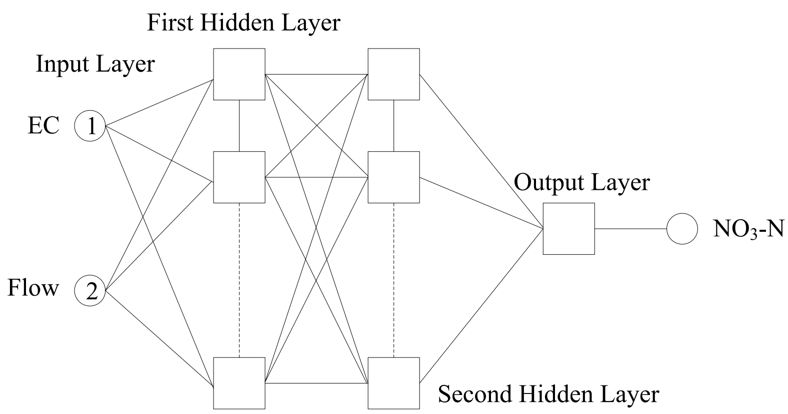

Figure 3. ANN model of the U-Tapao canal

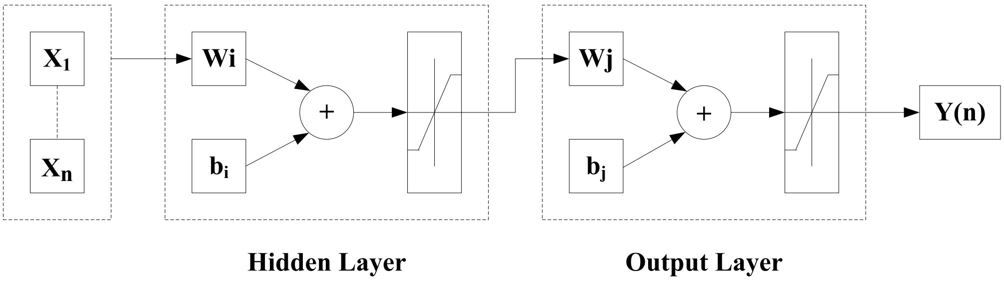

Figure 4. Generic FFBP architecture

2.4 Evaluation of the model performance

The correlation coefficient (*r*), coefficient of determination (R^2) and root mean square error (*RMSE*) were used to evaluate the performance of the models. The *r*, R^2 and *RMSE* criteria were calculated based on the following relationships:

$$r=\frac{n\sum xy-\sum x\sum y}{\sqrt{\left[n\sum x^2-\left(\sum x\right)^2\right]\left[n\sum y^2-\left(\sum y\right)^2\right]}} \quad (1)$$

$$R^2=\frac{(n\sum xy-\sum x\sum y)^2}{\left[n\sum x^2-\left(\sum x\right)^2\right]\left[n\sum y^2-\left(\sum y\right)^2\right]} \quad (2)$$

$$RMSE=\sqrt{\frac{1}{n}\sum(x-y)^2} \quad (3)$$

Where x is the measured concentration, y is the predicted concentrations, and n is the total number of datum.

3. Results and Discussion

The performance of the ANNs is presented in Table 3. Different ANN structures were constructed for the prediction of NO_3-N in the U-Tapao canal. The optimal ANN structure was selected as that which resulted in high values of *r*, R^2 and a low RMSE value in the training and testing.

The optimal ANN structure, with a low *RMSE* value and high values of *r* and R^2, was the four layer FFBP, with 2 neurons in the input layer, 20 neurons in the first hidden layer, 30 neurons in the second hidden layer, and a single neuron in the output layer with the tan-sigmoid transfer function (2-20-30-1). The respective values of *r*, R^2 and *RMSE* were: *0.937*, *0.878* and *0.514* for training, *0.849, 0.722* and *0.772* for testing, and *0.913, 0.833* and *0.714* for both training and testing combined. A plot of the relationship between the measured NO_3-N and the optimal FFBP model-predicted NO_3-N in both training and testing are shown in Fig. 6. The plot shows that the results are good for concentration lower than 3.0 mg/L of NO_3-N.

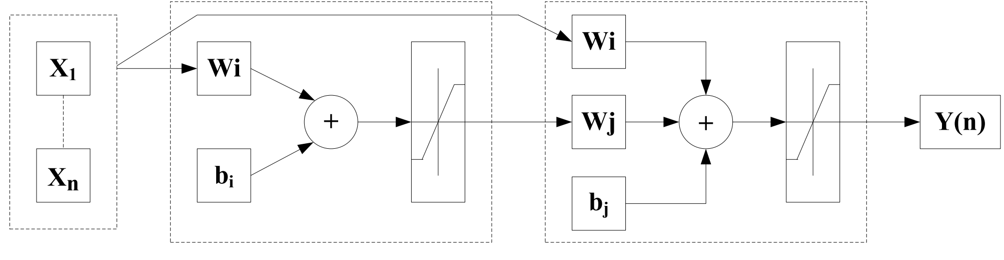

Figure 5. Generic CFBP architecture

Based on the performance of different transfer functions in the output layers shown in Table 3, the performance of the topologies of the tan-sigmoid transfer function are better than those of the log-sigmoid transfer function. The plot between the measured NO_3-N and the ANN model-predicted NO_3-N in training and testing are shown in Figs. 6, 7 and 8. Fig. 8 shows the results of the predictions of the optimal structure from the CFBP models (with the tan-sigmoid transfer function in the output layer), which are lower than the measured NO_3-N values.

The predictions of the NO_3-N with the tan-sigmoid transfer function in the output layer between FFBP and CFBP, are shown in Table 3. It can be seen that the performances of the three topologies (2-20-20-1, 2-20-30-1, 2-25-30-1) of the FFBP were superior to the performance of CFBP with only one topology (2-30-30-1) producing a comparable performance. Thus, it can be concluded that the FFBP model is the optimal ANN structure for the U-Tapao canal.

Table 3. Performance of FFBP, CFBP and linear regression models for prediction of the NO_3-N at UT16 station in the U-Tapao canal (Number of samples = 96 datasets)

Model	ANN Topology		Transfer Func. (Output) =tan-sigmoid			Transfer Func. (Output) =log-sigmoid		
			r	R^2	RMSE	r	R^2	RMSE
FFBP	2-30-30-1	Total	0.900	0.810	0.729	0.507	0.257	2.026
		Training	0.924	0.855	0.527	0.508	0.258	1.697
		Test	0.843	0.710	0.787	0.511	0.261	1.728
	2-25-30-1	Total	0.865	0.749	0.928	0.512	0.262	1.974
		Training	0.900	0.810	0.679	0.532	0.284	1.671
		Test	0.780	0.609	0.987	0.512	0.262	1.641
	2-20-30-1	Total	0.913	0.833	0.714	0.626	0.392	1.917
		Training	0.937	0.878	0.514	0.646	0.418	1.604
		Test	0.849	0.722	0.772	0.574	0.330	1.637
	2-20-20-1	Total	0.902	0.814	0.748	0.439	0.192	1.967
		Training	0.920	0.846	0.575	0.480	0.231	1.646
		Test	0.86	0.74	0.746	0.353	0.125	1.683
	2-20-10-1	Total	0.888	0.789	0.792	0.554	0.307	1.946
		Training	0.912	0.833	0.597	0.568	0.322	1.631
		Test	0.830	0.689	0.821	0.520	0.270	1.657
CFBP	2-30-30-1	Total	0.901	0.812	0.754	0.549	0.302	1.950
		Training	0.926	0.857	0.552	0.586	0.344	1.625
		Test	0.846	0.716	0.801	0.458	0.209	1.682
	2-25-30-1	Total	0.760	0.578	1.567	0.479	0.230	1.825
		Training	0.794	0.630	1.220	0.492	0.242	1.534
		Test	0.689	0.474	1.536	0.446	0.198	1.544
	2-20-30-1	Total	0.768	0.590	1.197	0.429	0.184	2.003
		Training	0.790	0.624	0.954	0.442	0.195	1.696
		Test	0.718	0.515	1.129	0.410	0.168	1.662
	2-20-20-1	Total	0.899	0.809	0.807	0.603	0.364	1.739
		Training	0.912	0.831	0.648	0.622	0.387	1.448
		Test	0.86	0.75	0.752	0.556	0.309	1.496
	2-20-10-1	Total	0.906	0.820	0.758	0.608	0.369	1.519
		Training	0.926	0.858	0.577	0.616	0.379	1.263
		Test	0.855	0.731	0.768	0.588	0.346	1.316
Linear Regression	NO_3 -N = (0.00938*EC) - (0.00227*Q) + 0.79153					0.845	0.714	0.829
	NO_3 -N = (0.01212*EC) + 0.12403					0.867	0.752	0.831

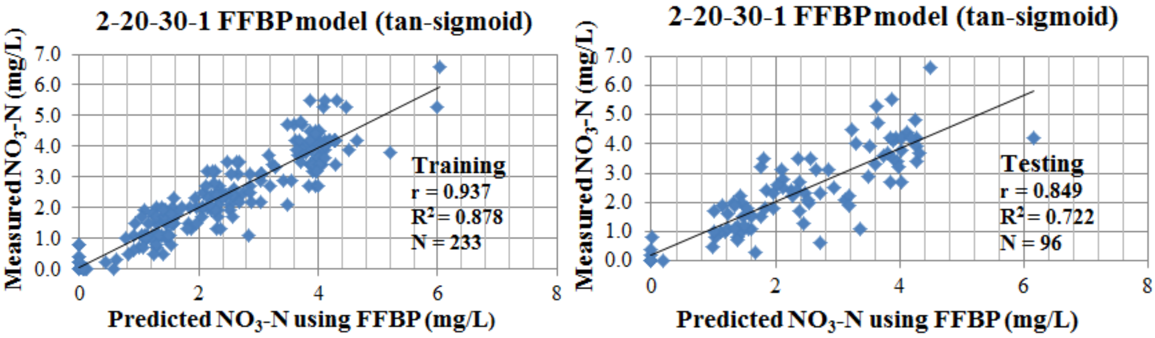

Figure 6. Comparison of the NO_3-N predicted by the FFBP model (with the tan-sigmoid transfer function in the output layer) and the measured NO_3-N in U-Tapao canal

In the past, EC was used to estimate nitrogen concentrations by developing a regression equation (Gali *et al*., 2012; Joarder *et al*., 2008). However, in the U-Tapao canal, flow rate is the highest negative relationship with NO_3-N. Therefore, EC and flow rate were selected to predict the NO_3-N by developing two linear regression equations. Table 3 and Fig. 9 illustrate the results of the linear regression analysis, which shows that the EC-only linear regression performance is superior to that of EC and flow rate linear regression.

The results of the linear regression analysis are also compared with the results obtained from the optimal FFBP model in Table 3, and Figs. 6 and 9. They show that the r, R^2 and *RMSE* values of the optimal FFBP model are superior to that from those achieved using regression analysis. The *RMSE* in the FFBP model is better than regression analysis by approximately 10 %. The two linear regression equations perform poorly for lower NO_3-N concentrations below approximately 1.5 mg/L. However, the FFBP model gives good predictions for lower NO_3-N concentrations. Therefore, the FFBP model was found by this study to be the most suitable structure to predict NO_3-N.

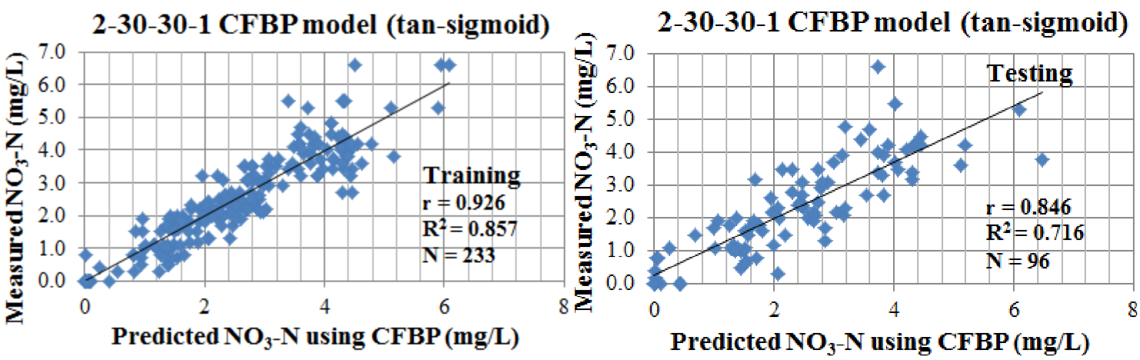

Figure 7. Comparison of the NO_3-N predicted by the CFBP model (with the tan-sigmoid transfer function in the output layer) and measured NO_3-N values in U-Tapao canal

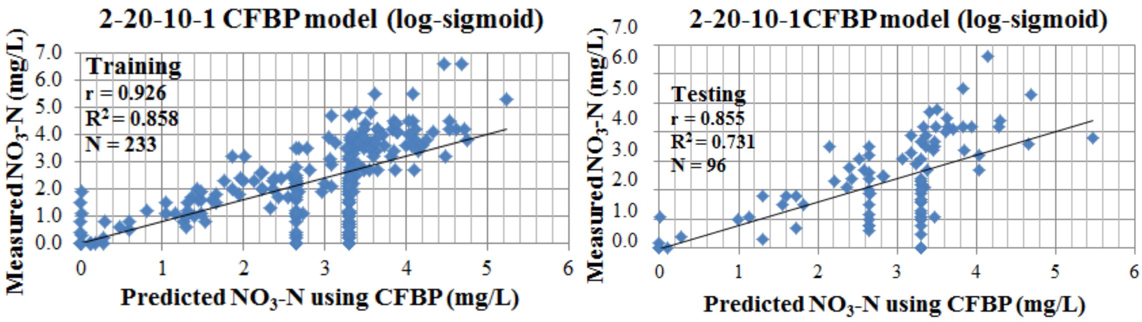

Figure 8. Comparison of the NO_3-N predicted by the CFBP model (with the log-sigmoid transfer function in the output layer) and measured NO_3-N values in U-Tapao canal

In this study, the optimal structure FFBP model (2-20-30-1) was validated. The *r*, R^2 and *RMSE* from the validation process were *0.930*, *0.864*, and 0.495, respectively. Fig. 10 shows the plots between the measured and model-predicted NO_3-N.

The time series comparison of the measured NO_3-N and the predicted NO_3-N obtained from the optimal ANN model is shown in Fig. 11. It can be observed that the NO_3-N concentration gradual increasing in the dry season (Feb.-Mar.), which was probably caused by decreased precipitation, as there was no rainfall in March 2015, causing low dilution. In addition, the U-Tapao canal is surrounded by agricultural land, factories, communities and urban areas and receives NO_3-N from point and nonpoint sources. For this reason, the level of NO_3-N and the flow rate have a negative relationship in this area. Similarly, the NO_3-N concentration was reduced to zero when there were high flow rates of between 400-750 m^3/s in the wet season (Dec.-Jan.), as shown in Fig. 2. This may be because residual nitrogen is flushed out during the first high flow event with the NO_3-N concentration gradually decreasing with over time during consecutive high flow events (Arheimer and Lidén, 2000).

4. Conclusions

In this study, two types of ANNs, FFBP and CFBP were developed to predict NO_3-N in the U-Tapao canal in southern Thailand with EC and flow rate being selected as the input data. Different ANN structures were constructed and tested and their performance was assessed based on *r*, R^2 and *RMSE*. The simulation results show that the application of FFBP for the prediction of NO_3-N is appropriate and reasonably significant for concentrations lower than 3.0 mg/L NO_3-N concentrations. Furthermore, the predictions of the FFBP model are better than that those obtained by linear regression analysis. Thus, FFBP can be used as an alternative tool for the prediction of NO_3-N concentrations in the U-Tapao canal. This approach may also be modified for use in other areas. In order to improve the accuracy of this prediction, the hypothesis of NO_3-N concentrations in the U-Tapao canal should be further spatially analyzed. Thus, artificial intelligence techniques such as ANN and the fuzzy logic are recommended to be combined with watershed models to form very effective tools for water quality prediction.

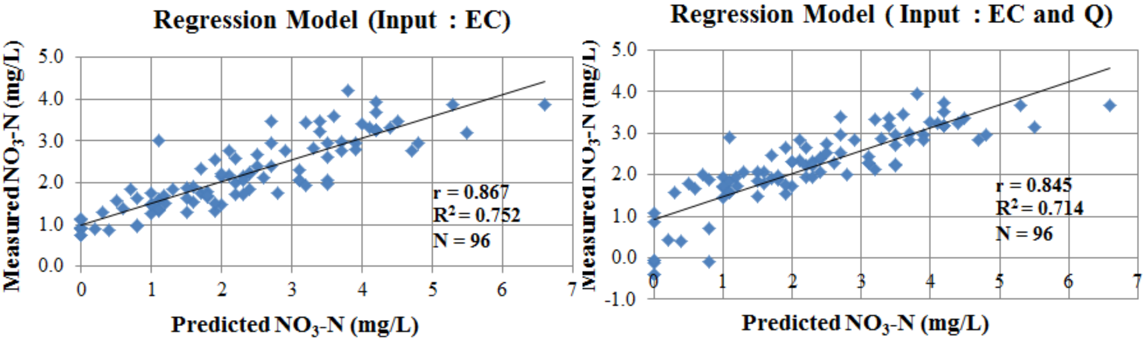

Figure 9. Comparison of the regression model-measured and the predicted NO_3-N values in U-Tapao canal

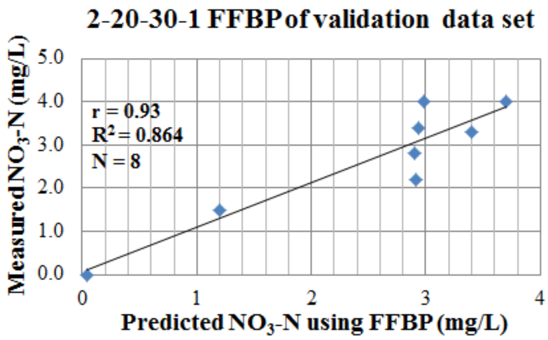

Figure 10. Comparison of the NO_3-N predicted by the 2-20-30-1 structure FFBP model and the measured values based on the validation data set (n = 8 samples)

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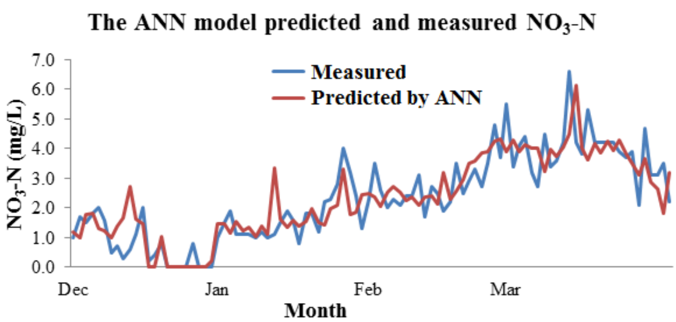

Figure 11. Comparison of ANN model-measured and predicted NO_3-N values in U-Tapao canal

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