Preprints of the 19th World Congress
The International Federation of Automatic Control
Cape Town, South Africa. August 24-29, 2014

Modelling of a coagulation chemical dosing unit for water treatment plants using fuzzy inference system ⋆

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Abstract: In this study, adaptive neuro-fuzzy inference system (ANFIS) was applied to estimate the parameters of a coagulation chemical dosing unit for water treatment plants. The dosing unit has three input variables (sudfloc 3835, ferric chloride and hydrated lime flow rates) and two output variables (surface charge and pH values). The ANFIS model is compared with multilayer backpropagation network (MBPN) with four different training algorithms for performance evaluation purpose. The results of evaluation tests using the average percentage error (APE), root mean squared error (RMSE), correlation coefficient (R) and average relative variance (ARV) criteria show that ANFIS is the most efficient and reliable estimator when the models were presented with noiseless and noisy input datasets.

1. INTRODUCTION

Coagulation in water treatment plants is a chemical and physical process that take place when coagulating chemicals are added to raw waters in a rapid mixing tank. The main objective is to aggregate micro-organisms, suspended and dissolved particles to form substances large enough to be separated by filtration or other related processes. Proper coagulation occurs when the quantity of coagulation chemicals added to the influent water streams is optimized. Thus, control of coagulation process is an essential aspect of water treatment operations that determine the overall success or failure of the portable water production [American Water Works Association & American Society of Civil Engineers , 2005].

Empirical modelling methods in the drinking water coagulation process have been discussed in the literature in the last few decades. Generally, researchers used linear regression, artificial neural networks, data mining and fuzzy inference systems to predict optimum coagulant dosages required for water treatment process. In one of the related studies, Baxter et al. [2002] developed a three-layer backpropagation network to predict the amount of alum dosage required to produce the desired quality of effluent water. In Wu & Lo [2008], the authors applied empirical modelling to polyaluminum chlorine dosage system by developing and comparing the performances of multilayer neural networks and adaptive neuro-fuzzy inference systems. Song et al. [2009] proposed a three-layer backpropagation model based on Levernberg-Marquard algorithm to predict the optimum coagulant dosage for water treatment plants.

These previous studies were focussed on modelling coagulant dosage-water quality parameters relationships. The models were developed to work with feed-forward control of coagulation process in the water treatment plants. However, they do not support development of feedback or multivariable control strategies that are necessary for correction of deviations from the system set points. In this study, fuzzy inference system is proposed to model the coagulation chemical dosing unit for water treatment plants. In particular, adaptive neuro-fuzzy inference system (ANFIS) was employed to model the unit. ANFIS has been reported to integrate the merits of artificial neural networks and fuzzy inference system into a single model. It has the ability to learn complex functional relationship between input and output dataset and accommodate hidden imprecision in the dataset and make accurate mapping accordingly. Thus, the preference for ANFIS over other empirical modelling techniques could be attributed to its fast computation and prediction performance abilities to describe the nonlinear characteristics of a system [Lohani et al, 2006, Zounemat-Kermani & Teshnehlab et al., 2008, Pai et al., 2009, Xiaojie et al., 2011].

Rietvlei water treatment plant in the City of Tshwane, South Africa was selected for the study. Historical data for a period of two years was collected from the plant. The performance evaluation of the ANFIS modelling technique was performed and compared with four variants of multilayer backpropagation network (MBPN) using statistical methods. This paper therefore demonstrates the suitability of fuzzy inference system for modelling a non-linear system such as coagulation chemical dosing unit of water treatment plants.

The paper is organised as follows. A brief description of the water treatment plant, coagulation chemical dosing

⋆ This work was supported by Tshwane University of Technology, Pretoria, South Africa.

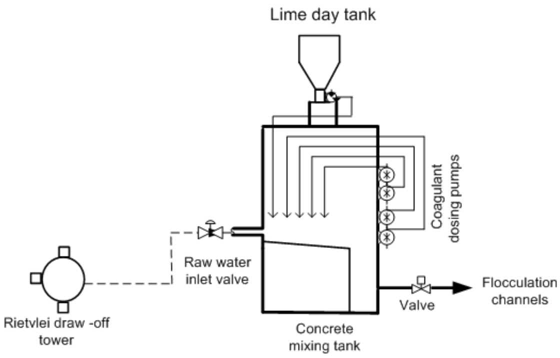


Fig. 1. Coagulation chemical dosing unit of Rietvlei water treatment plant

unit and fuzzy inference system are discussed in Section 2. Simulation results, discussions and performance evaluation of the model estimators are presented in Section 3. Finally, the concluding remarks are given in Section 4.

2. METHODS/MATERIALS

2.1 Water treatment process description at the Rietvlei water treatment plant

Rietvlei water treatment plant in the City of Tshwane, South Africa has a production capacity of about 40 million litres per day. The plant draws raw waters from Rietvlei dam located about 200 m away from it.

Fig. 1 illustrates the coagulation chemical dosing unit at the Rietvlei water treatment plant. It contains a concrete mixing tank with inlet and outlet channels. Sudfloc 3835, a blend of epichlorohydrin/dimethylamine (polyamine) and aluminium chlorohydrate [NSF, 2013] and ferric chloride solution are fed into the mixing tank as the coagulation chemicals. Calcium hydroxide (hydrated lime) in slurry form is also added to the mixing tank using a diaphragm pump to stabilise the water and adjust its pH value between 8.1 and 8.3.

The chemically treated waters flow out slowly and evenly through a series of baffled or flocculation channels, Dissolved Air Floatation/Filtration (DAFF) unit, Granular Activated Carbon (GAC) filtration unit and chlorination chamber before they are pumped to the storage reservoirs and distributed to final consumers [City of Tshwane, S.a].

2.2 Data Collection and Analysis

Historical data was collected from the plant for a period of two-year (2011-2012). A total of 690 data samples were successfully obtained from the daily operating records of the plant. The collected data were the flow rate of sudfloc 3835 solution (q_a), flow rate of ferric chloride solution (q_b), flow rate of hydrated lime (q_c) and the pH value of the effluent stream from the coagulation chemical dosing unit of the plant. The other variable of interest is the surface charge or streaming current of the treated water leaving the chemical dosing. It is an important variable for the implementation of multivariable or feedback control strategy for coagulation process in a water treatment plant [Evangelou, 1998, Adgar et al., 2005, Bello et al., 2013]. This was not measured presently at plant but was

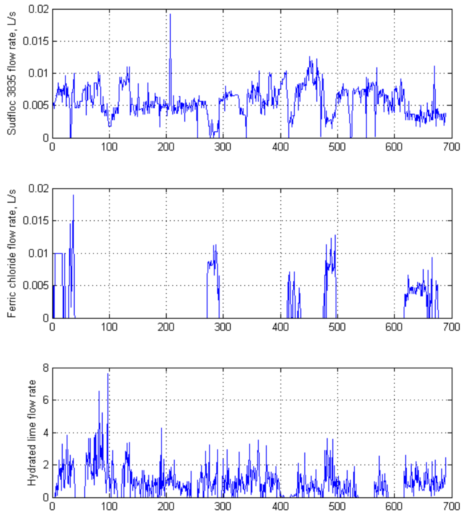


Fig. 2. Normalised input datasets for the models

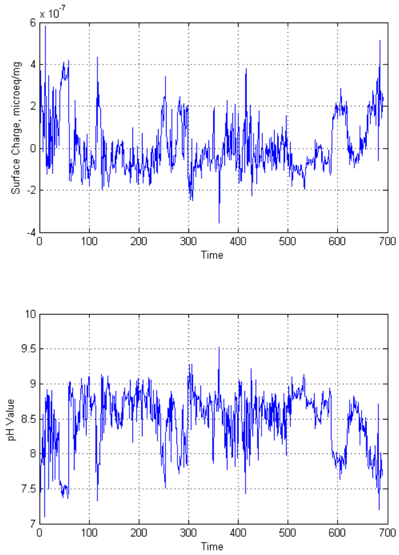


Fig. 3. Normalised output datasets for the model

computed using (1). Figs. 2 and 3 show the normalised data set used for modelling the coagulation chemical dosing unit.

$$\sigma = \left[\left(\frac{2}{\pi}\right) n\epsilon\kappa T\right]^{\frac{1}{2}} \sinh 1.15\,(pH_0 - pH) \qquad (1)$$

where σ surface charge, κ Boltzman constant, T temperature, ϵ relative dielectic permitivity, pH_o pH at point of zero charge and n ionic strength.

2.3 Adaptive Neuro-Fuzzy Inference System

Adaptive neuro-fuzzy inference system combines the fuzzy inference system into the framework of multilayer feed forward neural network. The general structure of the ANFIS is shown Fig. 4. The parameters associated with the input and the output membership functions are adjusted using gradient descent or hybrid algorithms. Consider a fuzzy inference system (FIS) with three inputs x_1, x_2, x_3 and one output f. For the first order Takagi-Sugeno fuzzy model, the fuzzy *if-then* rules are expressed as:

Rule 1: If x_1 is A_1 and x_2 is B_1 and x_3 is C_1, then $f_1 = p_1x_1 + q_1x_2 + r_1x_3 + s_1$

Rule 2: If x_1 is A_2 and x_2 is B_2 and x_3 is C_2, then $f_2 = p_2x_1 + q_2x_2 + r_2x_3 + s_2$

where A_1, A_2, and B_1, B_2 and C_1, C_2 are the membership functions for inputs x_1, x_2 and x_3 respectively; p_1, q_1, r_1, s_1 and p_2, q_2, r_2, s_2 are the parameters of the output membership functions.

Layer 1: Each node in this layer generates membership grade of an input variable. The node output OP_i^l is defined by:

$$\begin{aligned} OP_i^l &= \mu_{A_i}(x_1) \;\; for\, i = 1, 2\, or \\ OP_i^l &= \mu_{B_{i-2}}(x_2) \;\; for\, i = 3, 4\, or \\ OP_i^l &= \mu_{C_{i-4}}(x_3) \;\; for\, i = 5, 6 \end{aligned} \tag{2}$$

where x_1 (x_2 *or* x_3) is the node input, A_i (B_{i-2} *or* C_{i-4}) is the fuzzy set associated with this node, characterised by the shape of the membership functions in the node.
The membership function can be any of these functions: Gaussian; generalised bell shaped; trapezoidal shaped and triangular shaped functions. For a membership function that is a generalised bell function, the output of the node is obtained as:

$$OP_i^l = \mu_{A_i}(x) = \frac{1}{1 + (x - c_i/a_i)^{2b_i}} \tag{3}$$

where $\{a_i, b_i, c_i\}$ is the parameter set of the membership function with values in [0,1] interval.

Layer 2: Every node labelled as Π, in this layer multiplies all the incoming signals from the first layer. The output that represents the firing strength of a rule is expressed as:

$$OP_i^2 = w_i = \mu_{A_i}(x_1)\,\mu_{B_i}(x_2)\,\mu_{C_i}(x_3)\,, i = 1, 2, 3. \tag{4}$$

Layer 3: The i^{th} node of this layer, labelled as N, computes the normalised firing strengths as:

$$OP_i^3 = \overline{w_i} = \frac{w_i}{w_1 + w_2 + w_3} \tag{5}$$

where i = 1,2,3.

Layer 4: Node i in this layer computes the contribution of the i^{th} rule towards the model output, with the following node function:

$$OP_i^4 = \overline{w_i} f_i = \overline{w}_i\,(p_ix_1 + q_ix_2 + r_ix_3 + s_i) \tag{6}$$

where $\overline{w}_i$ is the output of layer 3 and $\{p_i, q_i, r_i, s_i\}$ is the parameter set.

Layer 5: The single node in the layer calculates the output of the ANFIS as:

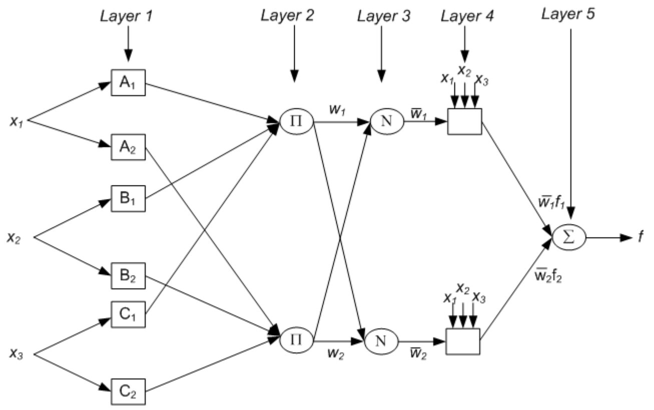


Fig. 4. ANFIS Architecture

$$OP_i^5 = \sum_i \overline{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i} \tag{7}$$

The overall output of the ANFIS architecture shown in Fig. 4 can be expressed as a linear combination of the consequent parameters:

$$\begin{aligned} f &= \frac{w_1}{w_1 + w_2 + w_3} f_1 + \frac{w_2}{w_1 + w_2 + w_3} f_2 + \frac{w_3}{w_1 + w_2 + w_3} f_3 \\ &= \overline{w_1} f_1 + \overline{w_2} f_2 + \overline{w_3} f_3 \end{aligned}$$

$$\begin{aligned} &= (\overline{w_1}x_1)\,p_1 + (\overline{w_1}x_2)\,q_1 + (\overline{w_1}x_3)\,r_1 + (\overline{w_1})\,s_1 \\ &+ (\overline{w_2}x_1)\,p_2 + (\overline{w_2}x_2)\,q_2 + (\overline{w_2}x_3)\,r_2 + (\overline{w_2})\,s_2 \\ &+ (\overline{w_3}x_1)\,p_3 + (\overline{w_3}x_2)\,q_3 + (\overline{w_3}x_3)\,r_3 + (\overline{w_3})\,s_3 \end{aligned} \tag{8}$$

Assuming the set of total parameters (T) can be separated into two such that T_1 denotes a set of antecedent parameters a_i, b_i, c_i and T_2 denotes the set of consequent parameters $\{p_i, q_i, r_i, s_i\}$. These parameters are adjusted using the hybrid learning algorithm, a combination of gradient descent and least-squares methods. The algorithm has forward and backward passes to identify or search for the optimal parameters of the ANFIS. In the forward pass, the consequent parameters are estimated by the least squares method. However, in the backward pass, the error rates propagate backward and the antecedent parameters are updated by the gradient descent method [Jang, 1993, Zounemat-Kermani & Teshnehlab et al., 2008].

2.4 Multilayer Backpropagation Network

Multilayer backpropagation networks (MBPN) are feedforward and static neural networks, made up of neurons (processing elements) and connections. They are arranged in three or more layers as follows: an input layer, hidden layer(s) and output layer[Yegnanarayana, 2005]. The layers in the network can use any combination of these nonlinear functions: log-sigmoid; tan-sigmoid and pure linear. The training of neural network involves presenting a set of input-output data to it. The weights and biases of the network are iteratively adjusted to minimize the average squared error between the network outputs and actual outputs. Different training algorithms for multilayer neural networks have been developed. Nearly all these algorithms determine how to adjust the weights by using the gradient of the performance function. Back propagation training

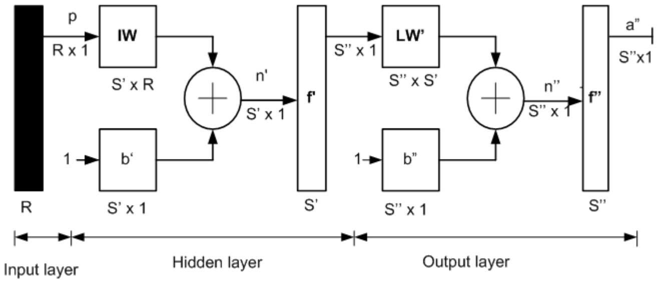


Fig. 5. Multilayer backpropagation network architecture

algorithm is a common technique to adjust the weight of multilayer neural network and minimise the performance function. There are several variants of this algorithm that have been discussed in the literature from low performance to high performance algorithms and heuristic to numerical optimization techniques. These several variations include: resilient backpropagation, conjugate gradient descent, Quasi-Newton and Levenberg-Marquardt algorithms[Hagan et al., 1996, Yegnanarayana, 2005].

Fig. 5 shows the architecture of a typical MBPN applied for this study.

The output of the MBPN is expressed as:

$$a^{'} = f^{'}\left(IWp + b^{'}\right) \tag{9}$$

$$a^{''} = f^{''}\left(LW^{'}a^{'} + b^{''}\right) \tag{10}$$

$$a^{''} = f^{''}\left(LW^{'}f^{'}\left(IWp + b^{'}\right) + b^{''}\right) \tag{11}$$

Where R is the number of input variables, p input vector, $a^{'}$ input vector to output layer, $a^{''}$ output vector, IW input weight matrix, $b^{'}$ bias vector of the hidden layer, $b^{''}$ bias vector of the output layer, $S^{'}$ number of hidden layer neurons, $S^{''}$ number of output layer neurons, $LW^{''}$ output weight matrix, $n^{'}$ input to the hidden layer transfer function, $n^{''}$ input to the output layer transfer function, $f^{'}$ hidden layer transfer function and $f^{''}$ output layer transfer function.

2.5 Performance Evaluation

The performances of ANFIS and MBPN models are evaluated using average percentage error (ARE), root mean squared error (RMSE), correlation coefficient (R) and average relative variance (ARV) (model efficiency) criteria. The expressions for these criteria are [Jang, 1993, Pai et al., 2009]:

$$APE = \frac{1}{N}\sum_{i=1}^{N}\frac{|y_i - \overline{y_i}|}{|\overline{y_i}|} * 100 \tag{12}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\overline{y_i} - y_i\right)^2} \tag{13}$$

$$R = \frac{\sum_{i=1}^{N}\left(y_i - \overline{y}\right)\left(\hat{y}_i - \overline{\hat{y}}\right)}{\sqrt{\sum_{i=1}^{N}\left(y_i - \overline{y}\right)^2 \sum_{i=1}^{N}\left(\hat{y}_i - \overline{\hat{y}}\right)^2}} \tag{14}$$

$$ARV = \left(\frac{RMSE}{s}\right)^2 \tag{15}$$

Where $\widehat{y}_i$ is the output of model estimator, y_i measured output, $\overline{y_i}$ mean of the measured output, (N) number of samples, s standard deviation.

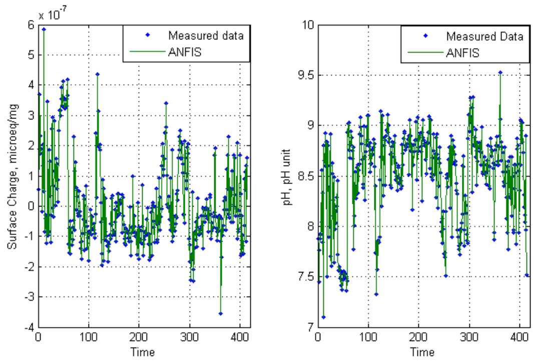
3. RESULTS AND DISCUSSIONS

The input-output dataset was used for the development of the ANFIS model of the dosing unit. The data was divided into two parts: the first part (60%) was used to train the model and second part (40%) was the checking dataset to validate the model.

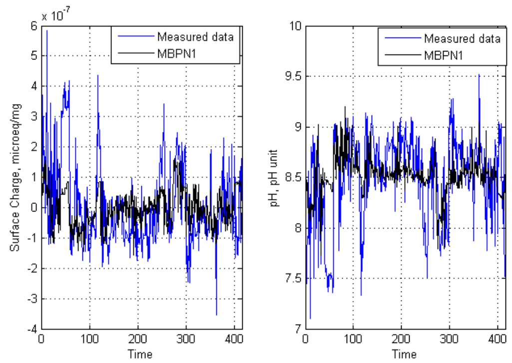
The ANFIS model was made up of two ANFIS networks. The first and second networks were developed to estimate SC and pH output variables respectively. The first network was trained with $[q_a - q_b - q_c - SC]$ dataset and the second network was trained with $[q_a - q_b - q_c - pH]$ dataset. Each dataset comprised of 414 data pairs. The two ANFIS networks had similar structure. Two generalised bell membership functions were used for each input variable of the network. Each output variable had eight linear membership functions. Each network had 8 fuzzy *if-then* rules and 50 fitting parameters that were made up of 18 antecedent parameters and 32 consequent parameters. The training epoch was set at 100.

For comparison purpose, four variants of MBPN models consisting of input layer with 3 neurons (coagulation chemical flow rates) and output layers with 2 neurons (SC and pH) were developed. The number of hidden layer neurons that achieved the desired performance level (13 neurons) was determined after several trials by varying the neurons between 10 and 30. The tan-sigmoid transfer function was used at the hidden layer and linear transfer function at the output layer. The weights and biases of the networks were adjusted using the resilient backpropagation (MBPN1), scaled conjugate gradient (MBPN2), Quasi-Newton (MBPN3) and Levenberg-Marquardt (MBPN4) training algorithms. The training epoch of the MBPN was set as 100.

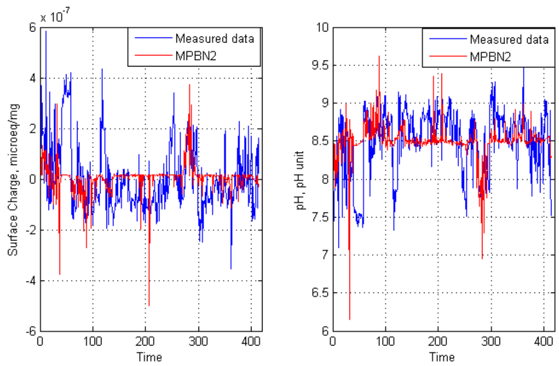
After the training of the ANFIS and four MBPN models, the validation simulation run was performed using the checking dataset consisting of 276 data pairs. The results of training and validation tests are shown in Figs. 6 and 7 respectively. These figures also indicate the comparison of the estimated output variables (SC and PH) from the ANFIS and MBPN models with the measured data. The performances of the ANFIS model and MBPN were compared using the evaluation criteria in (12)-(15). It can be seen from Tables 1 - 3 that ANFIS had the least APE, RMSE and ARV values when estimating both SC and pH from the training and checking datasets. In Table 4, the correlation coefficients of the models were compared. The ANFIS model has the highest correlation for both SC and pH estimations. In both cases, it took several simulation runs before four MBPN models converged to the final results. However, ANFIS converged faster and has a more consistent results than MBPN models. It is therefore inferred that it is more efficient than the MBPN models. This is confirmed by the consistent simulation results demonstrated by ANFIS between the training and checking datasets. The visual inspection of Figs. 6 and 7 show that ANFIS is a more preferable technique to model



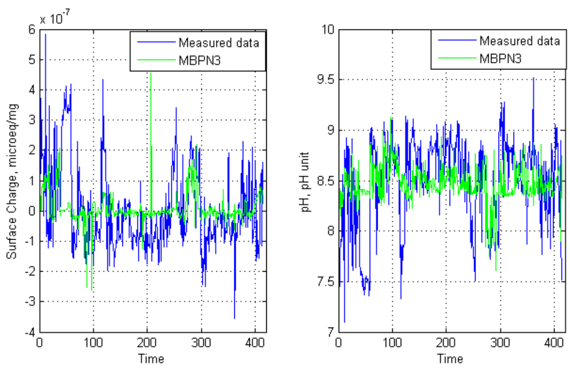
(a) Performance of ANFIS model



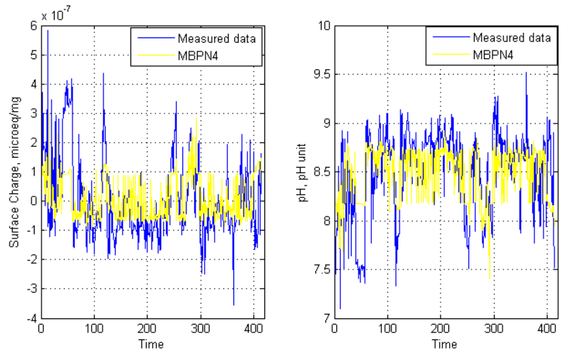
(b) Performance of MBPN1 model



(c) Performance of MBPN2 model



(d) Performance of MBPN3 model



(e) Performance of MBPN4 model

Fig. 6 Simulation responses of the models with the training dataset

Table 1. Performance Evaluation: APE, %

Model	SC_{trng} (10^{-4})	SC_{ckg} (10^{-4})	pH $_{trng}$ (10^{-4})	pH_{chkg} (10^{-4})
ANFIS	0.00001	0.00001	0.00001	0.00001
MBPN1	1.36	2.53	2.66	6.06
MBPN2	1.29	2.26	2.40	4.60
MBPN3	1.18	2.03	2.29	4.07
MBPN4	1.38	2.34	2.27	4.17

Table 2. Performance evaluation: RMSE

Model	SC_{trng} (10^{-7})	SC_{ckg} (10^{-7})	pH $_{trng}$ (10^{-7})	pH_{chkg} (10^{-7})
ANFIS	0.001	0.001	0.001	0.001
MBPN1	1.48	1.57	4.70	6.69
MBPN2	1.35	1.35	4.24	4.2
MBPN3	1.31	1.31	4.04	4.04
MBPN4	1.67	1.67	4.05	4.05

Table 3. Performance evaluation: ARV

Model	SC $_{trng}$	SC_{chkg}	pH_{trng}	pH $_{chkg}$
ANFIS	0.0001	0.0001	0.0001	0.0001
MBPN1	1.13	1.65	1.14	0.40
MBPN2	0.94	1.19	0.93	0.37
MBPN3	0.88	1.03	0.83	0.35
MBPN4	1.43	1.52	0.84	0.43

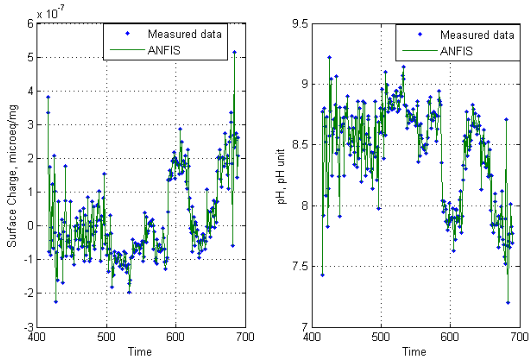
Table 4. Performance evaluation: R

Model	SC $_{trng}$	SC_{chkg}	pH_{trng}	pH_{chkg}
ANFIS	0.98	0.98	0.98	0.98
MBPN1	0.36	0.21	0.45	0.36
MBPN2	0.10	0.27	0.42	0.34
MBPN3	0.40	0.37	0.52	0.34
MBPN4	0.56	0.38	0.64	0.39

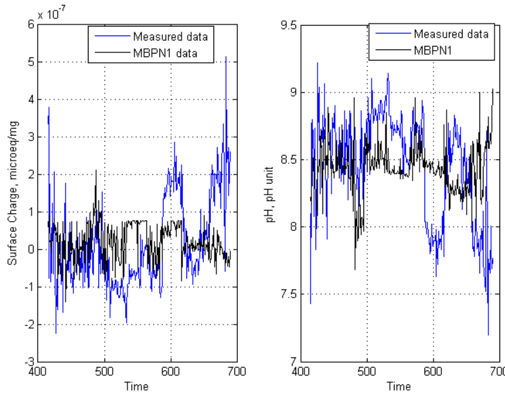
the chemical coagulation dosing unit of a water treatment plant than MBPN models.

In this part of the study, the checking dataset with noise signals were presented to the ANFIS and four MBPN model estimators. The responses of these model estimators under this condition was investigated and compared. The models were trained with the previous training datasets. After the training, the noisy checking dataset was presented to the models. The responses of each model were compared with the responses of the models with the previous checking dataset (without noise signal).

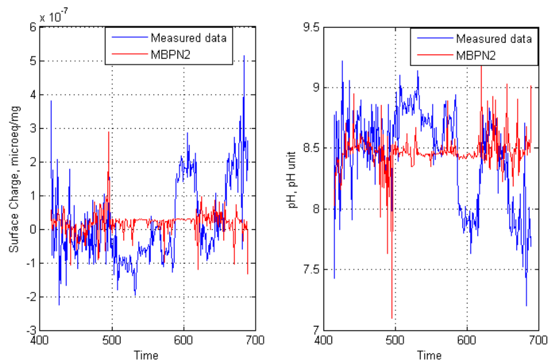
Figs. 8 shows the responses of each output variable of these models when two different checking datasets were presented to them. Visual inspection depicts that the responses of four MBPN models deviated significantly when presented with both noisy and noiseless checking



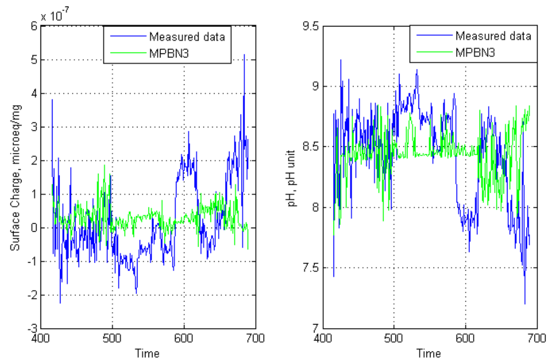
(a) Performance of ANFIS model



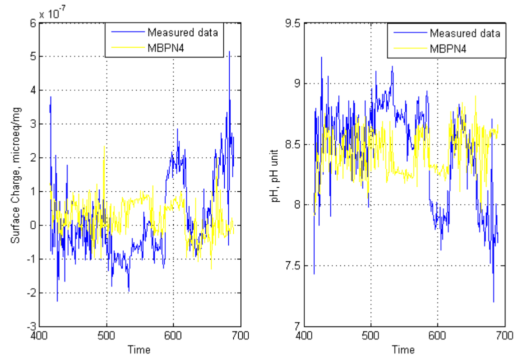
(b) Performance of MBPN1 model



(c) Performance of MBPN2 model



(d) Performance of MBPN3 model



(e) Performance of MBPN4 model

Fig. 7 Simulation responses of the models with the checking dataset

Table 5. Comparison of ARV for models with noisy and noiseless input checking dataset

Model	$SC_{noiseless}$	SC_{noisy}	$pH_{noiseless}$	pH_{noisy}
ANFIS	0.0001	0.0001	0.0001	0.0001
MBPN1	1.65	1.17	0.30	1.30
MBPN2	1.18	1.36	0.37	1.07
MBPN3	1.02	1.27	0.41	1.19
MBPN4	1.52	2.05	0.43	1.62

datasets. However, ANFIS had no significant deviation between the responses of the noisy and noiseless checking datasets. The ARV of each model was obtained and compared under the two distinct conditions. Table 5 shows the model efficiency (ARV) of the model estimators. It is seen from Table 5 that ANFIS has the least values. The results shows that ANFIS was able to filter out the added noise signals and estimated the model efficiently despite the addition of Gaussian noise to the input data of the models.

4. CONCLUSION

This study develops and compares models of adaptive neuro-fuzzy inference system and multilayer backpropagation networks for the coagulation chemical dosing unit of Rietvlei water treatment plant. Under different input conditions, ANFIS model was identified as an the most efficient estimator. It is further demonstrated the capabilities of ANFIS to filter out noise or disturbances over MBPN. ANFIS model is therefore a useful technique to build complex and nonlinear relationships, implement intelligent multivariable control strategies and optimise coagulation process in water treatment plants. The future work will include performance evaluation study between ANFIS modelling and data mining or evolutionary computation techniques.

ACKNOWLEDGEMENTS

The authors will like to thank Dr. Anish Kurien for his useful suggestions and comments. The cooperation of the management and staff of Rietvlei water treatment plant with respect to this research work is appreciated.

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