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Predicting TOC removal efficiency in hybrid biological aerated filter using artificial neural network

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ABSTRACT

The present study employs artificial neural network (ANN) models to forecast the total organic carbon (TOC) removal efficiency in biological aerated filter in a laboratory-scale reactor. This model is based on the measured values of TOC at inlet and outlet under different organic loading rates. One layer radial basis function (RBF) neural network and one layer multilayer perceptron (MLP) algorithm of ANN models were used to predict the TOC removal concentrations in the effluent. Data from experimental study (187 records) were employed for training and confirming the models. The best error on test samples was 0.032 for RBF and 0.026 and 0.027 for two methods of MLP (goal set and validation set), respectively. The ANN-based simulation model demonstrated accurate results for TOC removal and provided an efficient tool for estimating parameters in wastewater treatment processes.

Keywords: Biological aerated filter; Total carbon removal; Multilayer perceptron (MLP); Radial basis function neural network (RBFNN)

1. Introduction

The most important purpose of applying biological wastewater treatment is to remove the biodegradable pollutants (i.e. total organic carbon (TOC), phosphorus and nitrogen) before being discharged to the environment. From the environmental point of view, the release of untreated and/or inappropriately treated wastewater effluents contained with previously mentioned pollutants could damage the quality of water bodies, rivers in particular, and also harms aquatic organisms and human beings [1–5]. Because of the organic structure of most constituents of wastewater, carbon removal is the main aim of approximately all wastewater treatment processes. Therefore, to properly

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determine an effective wastewater process, examining the quantity of the organic compounds in the wastewater is of high importance.

The complexity of biological treatment mechanism in reducing biodegradable organic compounds (i.e. TOC, BOD, and COD) in traditional models demonstrates that there are limitations and difficulties in controlling the non-linear connections between influencing variables and optimal operating situations [6-8]. The current laboratory procedures used to determine the maximum capacity of the system for removing the pollutants are tedious, time-consuming, challenging, and costly; besides, to conduct such procedures, related experts and linear tools are required [8–12]. Comparing with the current methods, a more appropriate way of evaluating organic matter so as to increase plant performance is needed. In other words, developing robust, manageable, easier to use, and time-efficient models for predicting organic removal fluctuations and plant implementation under different situations could be very essential [8].

Over the last decades, artificial intelligence tools, particularly neural networks, have been paid more attention by the researchers. Based on the previously conducted studies in this regard, neural networks is a promising tool which is capable of learning from the available data to both facilitate and also enhance a particular process. About the advantages of artificial neural networks (ANNs), fewer time requirements, no mathematical descriptions, ease of simulating the models, ability to forecast with few experiments which allow the investigators to employ this method to obtain accurate and quick access to results can be mentioned [8,9]. By applying such tools, we are able to overcome the difficulties of predicting empirical techniques in water and wastewater sciences and offer a tighter fit to the variables than conventional models [10–14]. For instance, modeling a full-scale industrial wastewater treatment plant [15], predicting a refinery wastewater parameters [16], modeling of adsorption process of phenolic compounds [17], estimating the permeate flux during polyamide nanofiltration [18], using (ANN) for testing the efficiency of an assembled wetland [19]. Although many researches have demonstrated the benefits of the ANN system in water and wastewater treatment processes, few studies have applied ANNs in predicting TOC removal particularly from hybrid BAF (i.e. as one of the high-ranking approaches in carbonaceous).

The aim of the study is to explore the ability of two different ANN methods (radial basis function (RBF), multilayer perceptron (MLP)) for estimating TOC removal efficiency (as output quality parameter) of hybrid BAF reactor, illustrating the effect of specific

parameters on the network implementation, and selecting out noisy data, which are measured during the laboratory process. The best network model was revealed by indicating the proper network structure according to the number of radial basis points (centers) for RBF, the number of hidden neurons for MLPNN, the least error in comparison with real outputs (RMSE), the best type of transfer function. To prove the validity of this method, MLP NN was employed on goal and validation set, and was compared to RBFNN according to RMSE. In the present work, different linear and nonlinear transfer functions were tested for the hidden and output layers, also training data were fixed through construction of the best model. The results proposed here will be possible to be used in predicting the behavior of the essential factors of wastewater treatment, and determining the best amount of loadings and input and output parameters, which have a fundamental influence on the efficiency of WWT.

In this study, concerning the motivation and justification, there are some considerable issues which are focused on, including the importance of influent and effluent of TOC in wastewater treatment, how to develop the model accuracy according to the number of hidden neurons and the transfer function applied, and which method would probably perform better and why.

2. Materials and Methods

2.1. Experimental setup

The data used in this report were gathered from the hybrid BAF (partially packed reactor). The reactor was operated for 250 d in a controlled situation [20]. PVC biofilter, 100 cm in height and 14 cm in diameter, was separated into attached growth part (0.55 m) and suspended growth part by using a polypropylene mesh. The attached growth part (upper zone) was filled by plastic media cascade mini rings (Glitsch, UK). The schematic of the reactor and experimental equipment is shown in Fig. 1.

The synthetic wastewater consists of Whey Powder 16 g L⁻¹, Glucose 13.5 g L⁻¹, NH₄H₂PO₄ 1.915 g L⁻¹, NiSO₄·6H₂O 0.006 g L⁻¹, MoO₃ 0.0035 g L⁻¹, Meat extract 30 ml/at 200 g L⁻¹, and FeCl₃ 0.0225 g L⁻¹ was applied with respect to providing the main food resources containing carbon sources for microbial growth for all loadings [21,23]. Feeding was performed after 7 d of full internal recycling, with a very low organic loading rate (OLR) of 0.5-kg COD m⁻³ d⁻¹ to allow adaption of biomass to the new environment along with OLR and hydraulic loading rates stresses throughout the start-up stage [22]. COD tests were

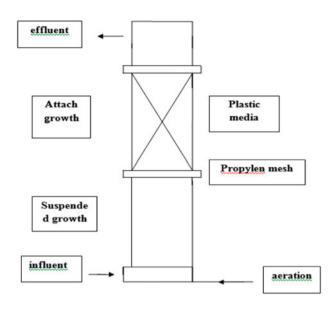


Fig. 1. The schematic of partially packed biological aerated filter.

performed to support the TOC removal rate in influent and effluent for each loading step. Increased COD loading rates were achieved by enhancing the influent's flow rate of $3.30-43.20 \text{ L} \text{ d}^{-1}$. The reactor was run until a stable condition performance (mean carbon removal) was attained. The reactor was backwashed with a regularity of once in every two or three days within the cycle of air scour, combination of air scour and water wash, rest and water wash with its own effluent to avoid the unusual organisms into the specific bacteria community [23].

Each effluent sample was gathered at the end of a sustained period of each loading of the BAF reactor and 1–4 h before the backwashing process. The effluent carbon removal (ETOC) was calculated based on TOC analyzer and according to related OLRs and the TOC removal efficiencies (TOC = TC – IC).

2.2. Development of the (ANN) model

2.2.1. Description of the input and output parameters

The most important factor to specifically determine and control the carbon concentrations in influent and effluent of the reactor is TOC. Since the computation of TOC in effluent depends on a variety of parameters such as pH, influent total organic carbon (ITOC), DO, and OLRs, an acceptable analysis of this substrate was determined by two specific factors, different ITOC and OLRs applied, which play an essential role in the wastewater treatment process. ITOC and OLR were employed to the model to simulate the ETOC using ANN.

2.2.2. Topology of ANN

An ANN is a mathematical modeling tool consisting of three layers of simulated neurons, input, output, and hidden layer, which are connected together by strength interconnections namely, weighted links in a variety of structures [24-26]. It provides the potential to model any nonlinear procedures by means of weighted connection sets [25]. The perception of utilizing ANN came from the human brain's structure, since the elements are known to perform as brain informational processing [27]. The best neural networks architectures can be considered as mapping from the most related input/output spaces and has a fundamental and essential concern to recognize appropriate predictors of the output and in detecting the optimal models, which is basically related to understanding the relationships between existing data [28].

Training data are conducted by training algorithms to fix the weights by reducing the error through cases in the training data-set [29,30]. During training process, input data are fed into the model from left to right to produce the simulated outputs. Each neuron in each laver is connected to every neuron in contiguous layers by multiplying by the connection weights [31]. The weights and biases are adapted and then computation is performed from input layer into output layer. The error values are then propagated to previous layers [32]. The sum of weighted inputs $(w_{mn} \times x_n)$ plus hidden layer bias b_m result in model outputs y_m and then activation function in the hidden layer allows the network to learn nonlinear relationships and predict an output. According to the mathematical model of network, the inputs are demonstrated by x_1 , x_2 , and x_n and the output by y_m . The weight factors associated with each neuron are represented by w_{m1} , w_{m2} , and w_{mn} [31,33]. A diagram of a neuron of MLPNN [34] is given in Fig. 2.

$$y_m = \tan\left(\sum_m^n \left(w_{mn} \times x_n\right) \pm b_m\right) \tag{1}$$

The data including inputs and output were normalized before the start of training, which can be described by Eq. (2):

$$X(n) = ((x - \min(x) / \max(x) - \min(x)))$$
(2)

To control and optimize the performance of the neural network architecture, the RMSE value (root mean square error) was investigated [35,36]. The following equation illustrates RMSE for different number of

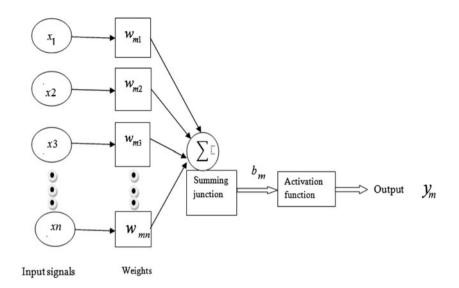


Fig. 2. Mathematical model of a neuron of MLPNN.

neurons in hidden layer. RMSE (Eq. (3)) is defined based on t_i and y_i which shows the desired and predicted outputs for *i*th sample, respectively.

RMSE =
$$\sqrt{\frac{1}{n}} \sum_{i=1}^{n} (y_i - t_i)^2$$
 (3)

2.2.3. ANN design for TOC removal prediction

In the current study, RBF and MLP architectures with three layers of neurons were used to estimate each constant function with an arbitrary accuracy. In order to reach the best learning condition as the main part of simulation, the network was trained many times with different number of training data-sets, different learning algorithms and different number of neurons in a hidden layer in order to obtain good prediction results (minimum error). Identifying proper training algorithm is a challenging and crucial issue for mapping MLP neural network models [37,38], and depends on such factors as complexity of the subject, the number of data and the position of training and test set [39]. Yetilmezsoy [40] investigated the advantages of using Levenberg-Marquardt algorithm in comparison with other algorithms, and found it particularly suitable as the best BP algorithm in accurate training.

Regarding the number of hidden layers and the neurons inside, many researchers suggest that one hidden layer containing some hidden neurons is adequate to obtain a reasonable result [37]. Afterwards, in the training phase, weights are calculated to minimize the network error function based on the chosen Levenberg–Marquardt learning algorithm, and root mean square error (RMSE) as the error function, tangentsigmoid (tansig) as a transfer function for input and hidden layer, a linear (purelin) as a transfer function for output layer, and the back-propagation gradientdescending method as the most popular learning algorithm. RMSE for the test data is calculated after each training set. The architecture of MLP used in this study is shown in Fig. 3.

In the current research, Neural Network Toolbox V4.0 of MATLAB[®] were employed to train 140 data (approximately 85% of total data) and test 19 observations (around 15% of total observations) to forecast the values of output (ETOC). In addition, EXCEL software was used for data information processing.

3. Results and discussion

3.1. Selection of MLP back-propagation (BP) algorithm using goal set and validation set

To predict the TOC removal using goal and validation set, a matrix of 140 samples was utilized for training and the best results were selected according to the least RMSE. To prevent overfitting of MLP neural networks, a validation set (10% of the main training samples as validation set and 90% as training set) was considered to determine the optimal number of hidden layer neurons and allow the model to make use of all existing data [31]. Table 1 reports the relationship between the number of hidden neurons and RMSE when a goal and validation set are considered.

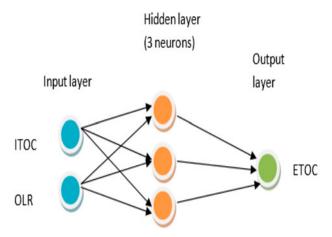


Fig. 3. Architecture of the best network for hybrid BAF reactor.

The results show that the best performance (minimum error on test set) was obtained when the

Table 1 RMSE on training and test set for goal and validation sets of MPLPNN

number of neurons in hidden layer is 9 and 1 for goal set and validation set, respectively. The following figure illustrates the network's performance regarding goal and validation sets of MLP.

According to Fig. 4, the network shows a reliable prediction except for the first and twelfth samples, which could be as a result of either the operator failure to record data or the apparatus failure. In the experimental laboratory test, the removal rate for each loading was calculated according to the mean TOC removal efficiencies and mean OLRs applied. Fatiha et al. revealed that partial bed appears to have a reasonable removal capacity at OLRs in the range of $3.0-5.0 \text{ kg COD m}^{-3} \text{ d}^{-1}$, with the percentage removal rate almost above 90% [23]. Therefore, an amount lower or higher than the one mentioned leads to such weakly predicted results. However, such data are assigned as chaotic variable (noisy data) and could be eliminated.

Train/test set	Num of hidden neurons									
	1	2	3	4	5	6	7	8	9	10
Training (goal)	0.010	0.010	0.010	0.010	0.010	0.010	0.010	0.010	0.010	0.010
Testing (goal)	0.032	0.036	0.034	0.033	0.032	0.033	0.036	0.034	0.029	0.033
Training (validation)	0.010	0.010	0.010	0.011	0.010	0.010	0.010	0.010	0.010	0.012
Testing (validation)	0.029	0.033	0.034	0.043	0.034	0.034	0.034	0.034	0.039	0.045

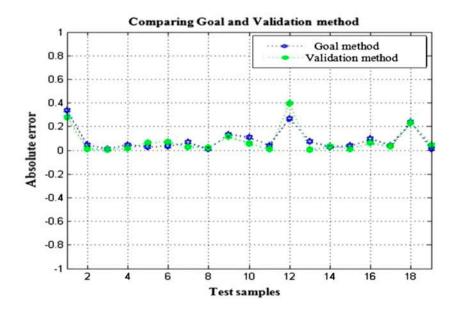


Fig. 4. Prediction error on test samples for goal set and validation set from left to right respectively.

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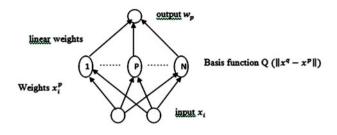


Fig. 5. The RBF structure.

3.2. Selection of RBF neural network for prediction of TOC removal

RBF with three-layer neural network has been the original method for performing specific function interpolation [41]. The first layer is input layer composing of the signal basis neurons. All neurons within the hidden layer demonstrate the value of the input model according to its hidden unit basis vector [25,42], which operates as a nonlinear transformation. The last layer is the output layer that contains linear nodes and replies to the position of imported patterns [25]. A random selection of a series of center values,

Table 2 RMSE on training and test set for RBF in Partial bed using fixed width RBFs, and training the weights into the linear output units is the simplest way to train RBF networks (Eqs. (4) and (5)). The exact interpolation of RBF is shown in Fig. 5.

Where x_i is the network input, the output vector is $y(w_p)$, and Q_n is the RBF. The network can attain subsequent mappings of the input and output to form a linear grouping of the basic functions [43]. The output is obtained to be a linear grouping of the basis functions:

$$f(x) = \sum_{p=1}^{n} w_p Q_n(||x^q - x^p||)$$
(4)

To make the equation simpler, we have:

$$Qw = t, \quad w = Q^{-1}t \tag{5}$$

RBF with different levels of spread has been used for TOC removal. Experimental data used in training and testing phases are needed for the development of the RBFNN model. Since constant spread considerably affects the predictive performance of the network (the larger the spread is, the smoother is the function

	Spread values									
Training and test set	0.1	0.3	0.5	0.7	0.9	1.1	1.3	1.5	1.7	1.9
Train set Test set	0.010 0.042	0.010 0.038	0.010 0.036	0.010 0.038	0.010 0.039	0.010 0.039	0.010 0.039	0.010 0.039	0.010 0.039	0.010 0.039

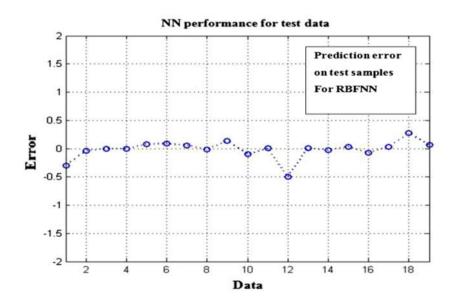


Fig. 6. Prediction errors of test samples in RBF network.

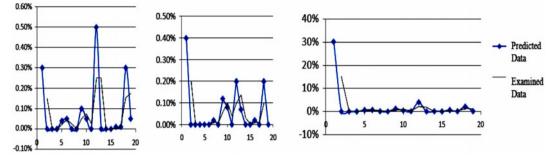


Fig. 7. Percentage error for all 3 methods; RBF, validation set MLP, and goal set MLP from left to right respectively.

Table 3 Comparison of RMSE in different methods

Method	RMSE			
RBF MLP (goal)	0.036 0.029			
MLP (validation)	0.029			

approximation), too large a spread means many neurons are required to fit a fast-changing function [42–44]. Too small a spread means many neurons are required to fit a smooth function, and the network might not generalize well. All the data, including inputs and output, were normalized between 0 and 1. Table 2 illustrates RMSE for training and test set for different spread values. The number of RBFs obtained for all spread values is equal to 1 and the goal was also set to 0.05. As Table 2 shows, the best spread is equal to 0.5 for this reactor.

According to Figs. 4 and 6, it is obvious that the same results in twelfth sample occur while training and testing the method, which is explained as a noisy and impaired data. Comparing all methods was performed by the percentage error (Fig. 7), RMSE (Table 3) as well as verifying real output and predicted output (Fig. 8). All three methods (RBFNN, goal, and validation set of MLP) demonstrate approximately equal results for all prediction methods. In general, the present study illustrated that feed-forward networks have performed slightly better than RBF.

The following figure shows the percentage error to determine the accuracy of this work. In this regard, the experimental values are compared with the predicted values in each three methods and showed reasonable and almost the same results for all methods, but a rather better result for MLPNN.

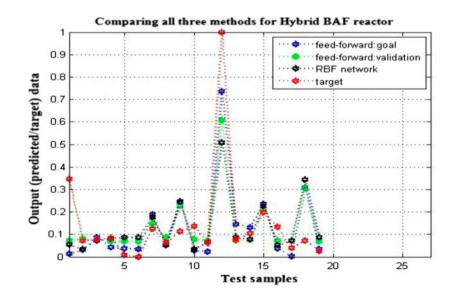


Fig. 8. Comparison of predicted models and real target outputs in a hybrid BAF reactor.

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4. Conclusion

Forecast models for TOC removal were developed using and comparing three topologies, RBF, goal set MLP and validation set MLP, containing one hidden layer in each structure. Feed-forward back-propagation (FFBP) with TRAINLM training algorithm, 1 hidden layer, 9 hidden neurons for goal set and 1 for validation set, TANSIG transfer function in hidden layer and PURELIN in output layer, were the end construct for MLP. Also three layer RBFNN with the best value of spread (0.5), Gaussian RBF and RMSE equal to 0.036 was obtained. The optimum networks were selected in terms of RMSE, number of epochs, and percentage error.

While RBFNN model performance was expected to indicate relatively more improved forecast, the results for the MLPNN and the RBFNN were not very far off and showed practically the same performance of those methods to predict accurately TOC removal concentration in the hybrid BAF reactor. In general, the present study showed that feed-forward networks performed slightly better than RBF.

The results revealed that the ANNs are a promising alternative to traditional linear forecasting processes to solve difficulties of predicting empirical techniques and will help to determine water and wastewater treatment processes [45] and estimate the influent annoyance to biological wastewater treatment plants. The findings of previous research and the opinions of other neural network experts are indicative of the fact that a hybrid network could be a logical solution. However, this might require several other control parameters as well as other soft computing alternatives such as a fuzzy neural network or a neural network associated with a genetic algorithm.

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