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APPLICATION OF ARTIFICIAL NEURAL NETWORKS FOR PREDICTING COD REMOVAL EFFICIENCIES OF ROTATING DISKS AND PACKED-CAGE RBCS IN TREATING HYDROQUINONE*

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Abstract– In this study, an artificial neural network (ANN) was applied to predict the performance of two rotating biological contactor (RBC) systems in removal of hydroquinone (a toxic aromatic compound). The first system was a two-staged conventional RBC and the second one was a one-staged packed-cage RBC with bee-cell 2000 biofilm carriers. Both systems had a total area of about 2 m^2 for biofilm attachment. The main aim is to predict COD removal efficiencies in both systems using ANN. Efficiency evaluation of the reactors was obtained at different influent COD from 200 to 5000 mg/L. Exploratory data analysis was used to detect relationships between the data and the evaluated dependents. The appropriate architecture of the neural network models was determined using several steps of training and testing the models. The modeling results showed that there is a good agreement between the experimental data and the predicted values with a correlation coefficient (R^2) of 0.998 and 0.997 for RBC with rotating disks and packed-cage RBC, respectively.

Keywords– Hydroquinone, COD, rotating biological contactor, neural networks

1. INTRODUCTION

Phenolic compounds are aromatic molecules containing a benzoic ring connected to one or several hydroxyl groups. These compounds are produced, consumed, and discharged to the environment by many industries [1]. Hydroquinone is one of the most important phenolic compounds, and it is widely used in agricultural, photographic, cosmetic, rubber and chemical industries. Hydroquinone can be treated by different physical and chemical methods such as adsorption, phenton, chemical oxidation and electrochemistry [2]. Previous studies indicate that it is also a biodegradable compound. For example, hydroquinone was oxidized with hydrogen peroxide and an enzyme extracted from a bacterium named *Serratia marcescens AB90027* as a catalyst. The results showed 96% removal in influent COD of 3500 mg/L [3]. In a different research, various pure cultures of microorganisms were tested to utilize hydroquinone as the sole carbon source. The pure cultures were isolated from soil, photographic and laboratory sludge, 97.5% total organic carbon (TOC) removal was gained after five days [4]. In another study, three phenolic compounds including pyrogallol, phenol and hydroquinone were investigated using Moving Bed Biofilm Reactor (MBBR) with polyethylene biofilm carriers. Hydroquinone had the highest removal efficiency of 90% for 700 mg/L influent COD [5].

The rotating biological contactor (RBC) usually consists of a series of plastic circular disks (biodisk). These disks are staged on a horizontal shaft, rotating perpendicular to the direction of the wastewater flow,

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and usually 40–45% of the total disk area is immersed in the wastewater. The attached microorganisms (biofilm) are alternatively submerged in the wastewater with the rotation of the disks. The biodisk is rotated at a speed which enables the development of the attached biofilm. Oxygen transfer is achieved by exposure and renewal of air–water interfaces, as the wastewater lifted out by the rotating device trickles back down into the tank. This cycle also benefits the adsorption and uptake of organics from the wastewater [6].

The RBC system has many advantages such as relative low energy consumption, simple operation and maintenance, and successive removal of the influent contaminants. This system has been successfully used in aerobic treatment processes such as decolorization [7], Fe oxidation, pathogenic bacteria removal from wastewater and nitrification [6]. This system has also been used in bioremediation of landfill leachates [8], heavy metals [9], and treatment of effluents from wineries [10], bakeries [11], food processing [12] and other biodegradable industrial discharges.

RBC systems have evolved significantly from the original design of several rotating discs. Many variations now exist, ranging from simple flat discs through corrugations to cellular meshes, all of which are designed to give extra surface area per unit volume [13].

Some alternations of RBCs media have been investigated at a laboratory-scale with satisfactory results of substrate removal. In one study, the disks of the RBC were modified by adding porous netlon sheets to increase area and volume of biofilm [14]. In another study, a layer of polyurethane foam was added on the discs to improve attachment of filamentous organisms [15].

Random packed media have been successfully tested as replacements for conventional disks at the laboratory and pilot-scale studies, providing extra surface area per unit volume. As a result, mass transfer efficiency will increase because of higher turbulence in the reactors. Also, the cost of fabrication of these systems is about one third that of conventional RBCs consisting of discs and their energy consumption is lower [16, 17]. Different kinds of packing such as pallrings, saddles and, cylindrical plastic elements with different sizes have been used in random packed RBC systems with satisfactory results [11, 17, and 18].

In a Biological wastewater treatment system like RBC, the performance of the system might have been influenced by influent characteristics variability. Therefore, biological process modeling is a demanding task as most of the available models are just approximations based on probabilities and assumptions. Recently, artificial neural networks (ANNs) have been increasingly applied in environmental and water resources engineering area [19].

The artificial neural network is a promising computational technique for modeling complex relationships, especially where the definite form of the relation between the variables is unknown. The advantages of ANNs are, less time required for model development than the traditional mathematical ones, ability to predict with limited numbers of experiments and their power to learn complicated relationships without knowledge of the model structure or phenomena involved in the process [20].

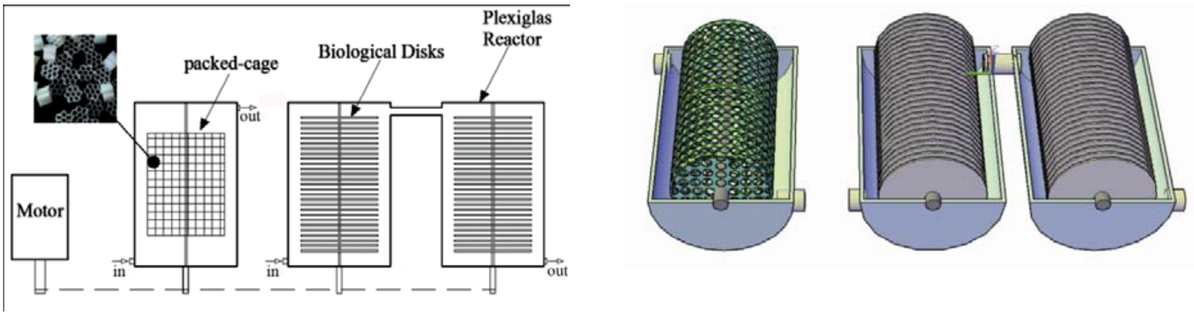
The first wave of interest in neural networks emerged after the introduction of simplified neurons by McCulloch and Pitts in 1943. More of ANN's history and a comprehensive review of their industrial applications can be found in the papers of Patterson and Meireles [21, 22]. ANNs have been applied to solve environmental engineering problems such as biological and physico-chemical wastewater treatment [23-26].

The main aim of this study is to compare the performance of conventional and packed-cage RBC biological systems in the treatment of wastewater containing hydroquinone and to develop models for predicting COD removal efficiencies using artificial neural networks.

2. MATERIALS & METHODS

a) Reactor setup

In this study, the removal efficiency of hydroquinone was investigated in two different laboratory scale RBC systems. The first system was a two-staged conventional RBC with rotating discs (RBC I and RBC II), and the second was a one-staged packed-cage RBC with bee-cell 2000 biofilm carriers provided by GRM (Global Resources Management) Company. Each stage of the rotating discs RBC consisted of 27 parallel plexiglas rotating disks (15 cm in diameters). The packed-cage RBC had a net drum full of biofilm carriers with specific surface area about 650 m^2/m^3. Both systems had a total area of 2 m^2 and were fed by a peristaltic pump. The schematic plan of the pilot and the 3-D view of the reactors are presented in Figs. 1a and 1b, and their specifications are summarized in Table 1. The specifications of bee-cell 2000 biofilm carriers are summarized in Table 2.



a) b)

Fig. 1. a) Schematic plan of the pilot b) 3-D view of the reactors

Table 1. Specification of the systems

Parameter	Conventional RBC	Packed-cage RBC
No. of stages	2	1
Volume of each stage (L)	3	3
Submergence (%)	40	40
Total biofilm area (m^2)	2	2
No of disk in each stage	27	-
Disks diameter (cm)	15	-

Table 2. Specifications of biofilm carriers in packed-cage RBC

Type	Bee-cell 2000
Material	Compressed polystyrene
Special area (m^2/m^3)	650
Quantity in 1 m^3	361000

Hydroquinone supplied by Merck Company served as the sole carbon source. To have C/N/P = 100/5/1, necessary nutrients (urea, KH_2PO_4, K_2HPO_4) were also added as supplement feed to the reactors in all experiments. Other compounds of the synthetic wastewater were (mg/L): $MgSO_4{\cdot}7H_2O$, 20; $FeCl_3$, 0.12; $CaCl_2$, 1.9; $MnSO_4$, H_2O, 2.5.

RBC samples were collected from the head-end of the first stage, and the tail-ends of all stages through the respective sampling ports placed in each stage of the reactor. The samples were filtered through a 0.45 μm Whatman filter paper. Chemical oxygen demand (COD) and hydroquinone concentration was measured daily for the influent and effluent from the stages during the period of operation. Analytical procedures followed in this study were those outlined in Standard Methods, for example, the COD experiments were based on the procedure code 5220 of this book [27]. Table 3 presents some of the equipment used in the experiments.

Table 3. Some of the equipment used in the experiments

COD Reactor:	Hatch DRB200
Spectrometer:	Lambda EZ 150
pH Meter:	Metrohm 691
Centrifuge:	Sigma 101
NMR 500:	AC-500MHZ (Bruker)

During the startup, the sludge seed was obtained from Ekbatan wastewater treatment plant which is located in the capital city of Tehran. In this period, the daily dosage of 200 mg/L COD as glucose and synthetic wastewater were fed to each reactor (for 60 days). After increasing biofilm mass, the acclimation was started with the stepwise substitution of glucose with hydroquinone ($COD_{hdroquinone}/COD_{total}$ was increased about 10% in each step). In this stage, the maximum removal efficiencies were 94, 94 and 92 percent, respectively for the first and second stages of RBC with rotating discs and packed-cage RBC in $COD_{hdroquinone}/COD_{total} = 0.5$. After the acclimation stage, the amount of COD was being increased stepwise up to 5000 mg/L. The duration of the reactor operation in the startup, acclimation and loading stages is shown in Fig. 2.

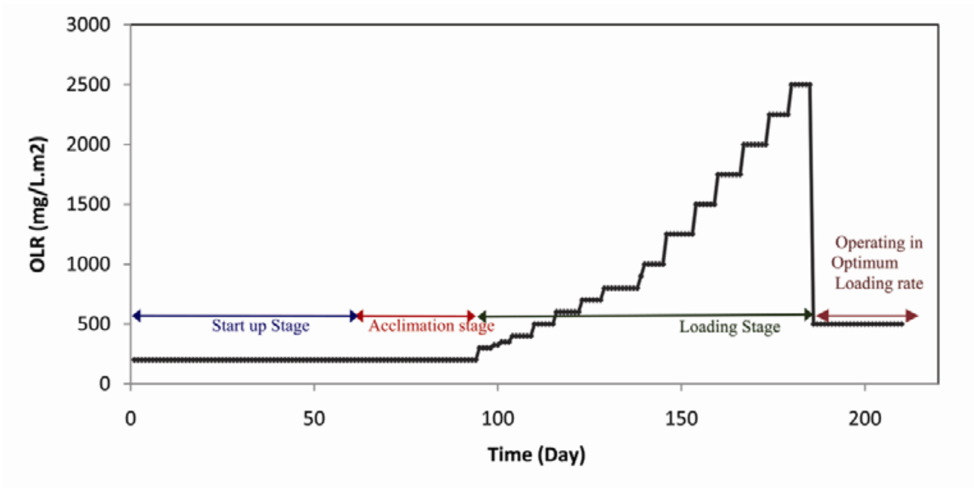


Fig. 2. Duration of reactor operation in different stages of the study

b) Software

For the development of the ANN models, Neural Network Toolbox 5 and MATLAB 9 (The Mathworks Inc. USA) were used. A MATLAB script was written which loaded the data file, trained and validated the networks. The input and output data were normalized and de-normalized for application in the network. A computer with a Core™2 Duo 2.5 GHz processor and 2 GB internal memory took a few seconds for processing of each neural network.

c) Neural networks

A neural network model consists as a set of parallel inter-connected simple computational units, called neurons. A neuron (also known as node) is a non-linear algebraic function, parameterized with boundary values [28].

Input-target training data are normally used to improve the optimization and behavior of the training process. Thus, the data are usually divided into three subsets; training, validation and testing. The training data are used for network learning and adjusting the network weights by minimizing an appropriate error function. Backpropagation is a training technique generally used for this purpose, and is a method for computing the gradient of the case-wise error function with respect to the weights for a feed forward network. The performance of the networks is compared by evaluating the error function using the validation subset data, independently. The test data are used to evaluate the generalization of the network and the accuracy of the targets for inputs, which are not in the training set [29].

-Selection of database: Selection of data for training the models is a very important step of developing each neural network. So, it must be done with a large and comprehensive set of reliable experimental data. In this work, the database was continuously collected for three months from the two systems. Reactors were fed with hydroquinone synthetic wastewater at a hydraulic loading rate of 1.5 $L/m^2.d$ and rotation speed of 5 rpm for disks and the packed-cage. COD removal efficiencies of each system were evaluated at different influent COD from 200 to 5000 mg/L. A total of 96 data pairs have been obtained from the experimental database and 70% of them were used as the training data. The rest of the data (30%) was used for validation and testing of the data.

-Selection of model architecture: Choosing the network structure is a very important step in the design of neural networks. The structure must be optimized to decrease computer processing time, obtain good performance and prevent overfitting. The number of input and output neurons is equivalent to the number of input and output data (respectively 3 and 1 in this study). Because of the many contributing factors, there is no definite way to determine of the best number of hidden layers and the optimum number of nodes in each layer. For example, the size of the training data set, the amount of noise in the targets, complexity of the sought function to be modeled, type of activation functions used and the training algorithm all affect the sizes of the hidden layers. The best number of hidden units cannot be determined without training several networks and estimating the generalization error of each. Thus, they are usually selected via a trial and error procedure [29].

Flood and Kartam [30] reported that use of more than one hidden layer provides more flexibility and enables estimation of more complicated functions with fewer nodes. According to Baughman and Liu's findings [31], adding the second hidden layer enhances the network prediction. Additionally, it was observed that, by adding the third hidden layer prediction capability is similar to a two hidden layer model, but it causes complexity of the structure and longer training times. Anderson and McNeill [32] suggested that the maximum number of neurons in the hidden layers can be estimated by dividing the number of input–output pairs in the training set by the total number of input and output nodes in the network multiplied by a scaling factor between 5 and 10.

In this study, the optimum number of hidden layers and nodes in each layer were determined using two nested for/next loop, one for setting the number of neurons in the first hidden layer and another for neurons in the second hidden layer. The best results were acquired with a three-layer network consisting of two hidden layers (Both had six nodes), and an output layer. The geometry of this network is illustrated in Fig. 3.

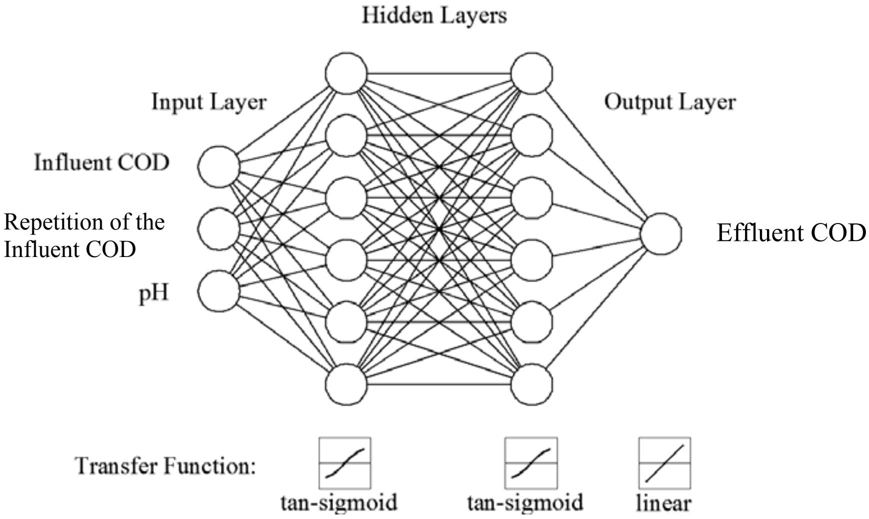


Fig. 3. Structure of the neural network model

-Back-propagation neural network: One of the best ways of training or determining the weights of the network is using back propagation strategy, which gives reasonable results with inputs that have never been exposed to the network. Standard backpropagation is a gradient descent in which the network weights are moved along the negative of the gradient of the performance function [33]. This method is used to distribute the error to achieve the best fit. An output is predicted by the network in a forward direction; then, the backpropagation algorithm redistributes the error of the resulted output back through the model, and weights are adjusted. The error is minimized through several iterations. Each complete cycle is called an 'epoch'. In each layer, all neurons are connected to every neuron in the next layer [34].

Based on the application and network architecture, the learning rate can be a crucial factor in the convergence of the neural network. This parameter can be used to decrease the chance of the training process being trapped in a local minimum instead of a global minimum [35]. A greater learning rate means a larger step. If the learning rate is extremely large, the algorithm will become unstable. On the other hand, an algorithm with a very small learning rate needs more time to converge. Momentum is a parameter which enables the network to respond to the local gradient and recent trends in the error surface. Moreover, a network without a momentum is vulnerable to the risk of getting stuck in a shallow local minimum [36]. In this study, the learning rate, maximum number of iterations, the momentum constant and the error goal were defined 0.001, 30, 0.8 and 0.01, respectively.

10 BP algorithms were compared to select the best fitting BP that minimized the error between neural network output and target value. For all algorithms, a three-layer network with a tan-sigmoid transfer function within the two hidden layers and a linear transfer function within the output layer were used. In order to determine the degree of error of trained model, testing and validation were used. In this study, the performance of the training was evaluated in terms of the mean square error (MSE) and determination coefficient (R), which determines the closeness of prediction between the desired and the predicted output from the neural network. After choosing the optimum BP algorithm, the number of neurons was optimized while other parameters were constant.

3. RESULTS & DISCUSSION

a) Experimental results

Variation of COD removal efficiencies of both rotating discs and packed-cage RBCs in influent CODs from 200 to 5000 mg/L are presented in Fig. 4. In these experiments, both systems were operated in a hydraulic loading rate of 1.5 L/m^2.d, and rotation speed of 5 rpm. In both systems COD removal efficiencies increased with raising COD up to 1000 mg/L. The highest COD removal efficiencies in RBC I and RBC II were 90 and 93 percent, respectively at COD=1000 mg/L. Packed-cage RBC had the highest COD removal efficiency of 88% in influent COD range of 700 to 1000 mg/L. For influent COD 1000-5000 mg/L, increasing the loading rate resulted in decreasing COD removal efficiencies in both systems. Up to 4000 mg/L influent COD, the RBC with rotating discs had higher removal efficiencies (about 5 to15 percent), but at higher loading rates, packed-cage RBC had better results.

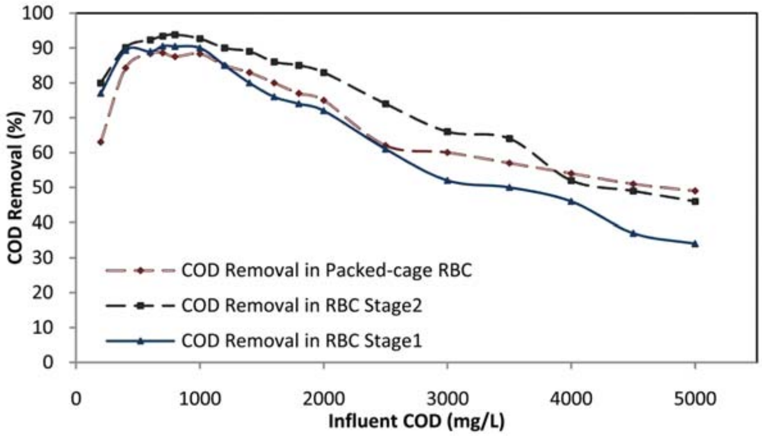


Fig. 4. Variation of COD removal in rotating disks and packed-cage RBC

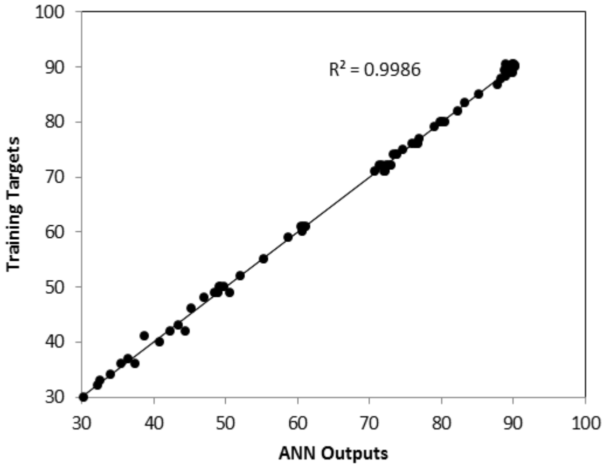
b) ANN model results

-Selection of backpropagation training algorithm: To determine the best backpropagation (BP) training algorithm, 13 BP algorithms were studied. Tangent sigmoid transfer function (tansig) at hidden layer and a linear transfer function (purelin) at output layer were used. In addition, 6 neurons were used in the hidden layers for all BP algorithms. Table 4 shows a comparison of different backpropagation (BP) training algorithms. Levenberg–Marquardt backpropagation algorithm (LMA) was able to have the smallest mean square error (MSE) and determination coefficient (R), compared to other backpropagation algorithms. Therefore, LMA was selected as the training algorithm in the present study.

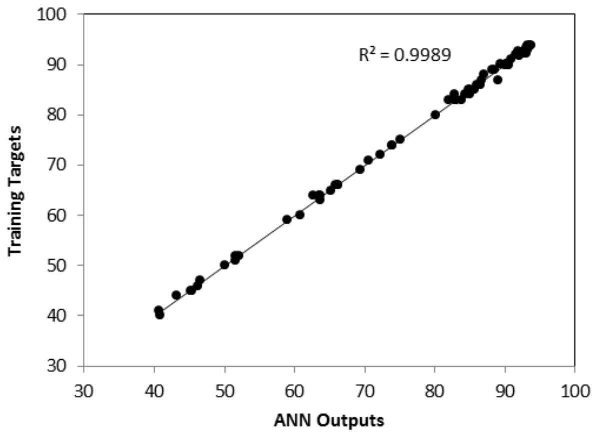
Table 4. Comparison of 13 backpropagation algorithms for predicting COD removal efficiency

Function	Back propagation (BP) Algorithm	RBC with rotating discs Stage 1			RBC with rotating discs Stage 2			Packed-cage RBC		
		MSE	R	Iteration	MSE	R	Iteration	MSE	R	Iteration
trainb	Batch training with weight and bias learning rules	40.479	0.94678	100	41.454	0.92511	100	38.745	0.95271	100
trainbfg	BFGS quasi-Newton BP	1.445	0.93723	100	1.452	0.94989	84	2.33	0.96774	86
trainbr	Bayesian regularization	2.884	0.99794	64	1.539	0.99811	100	1.671	0.99806	65
traincgb	Powell-Beale conjugate gradient BP	4.397	0.61969	100	3.798	0.36699	80	3.944	0.85117	100
traincgf	Fletcher-Powell conjugate gradient BP	10.257	0.17509	50	8.907	0.61735	49	9.478	0.7518	84
traincgp	Polak-Ribiére conjugate gradient BP	2.131	0.54888	95	2.92	0.82188	97	3.882	0.56599	96
traingda	Gradient descent with adaptive learning rule BP	15.707	0.98174	100	13.77	0.98006	100	15.744	0.096498	100
traingdm	Gradient descent with momentum BP	12.816	0.98604	100	11.333	0.98299	100	13.814	0.97164	100
traingdx	Gradient descent with momentum and adaptive learning rule BP	5.3431	0.99305	100	7.45	0.98955	100	7.081	0.98575	100
trainlm	**Levenberg-Marquardt BP**	**0.516**	**0.99931**	**100**	**0.297**	**0.99977**	**68**	**0.509**	**0.998931**	**100**
trainoss	One step secant BP	5.339	0.24688	100	5.918	0.78384	100	5.046	0.69911	87
trainrp	Resilient BP (Rprop)	6.46	0.99153	100	5.793	0.99181	60	8.496	0.99026	40
trainscg	Scaled conjugate gradient BP	3.822	0.99696	96	4.279	0.99317	100	2.53	0.9946	100

-Regression analysis: A regression analysis of the network response has been performed for the network output and the corresponding target (Fig. 5). Considering the non-linear dependence of the data, the output appears to track the targets reasonably well. Correlation coefficients (R^2) were 0.998, 0.998 and 0.997, and the obtained mean square error values were 0.516, 0.297 and 0.509 for predicted COD removal efficiencies in the first and second stages of RBC with rotating disks and packed-cage RBC, respectively.



(a)



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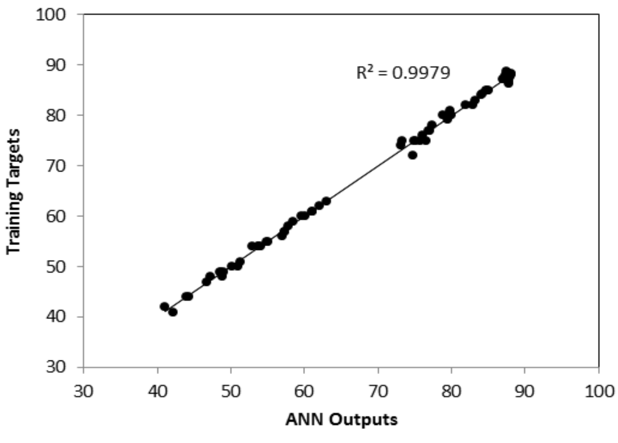
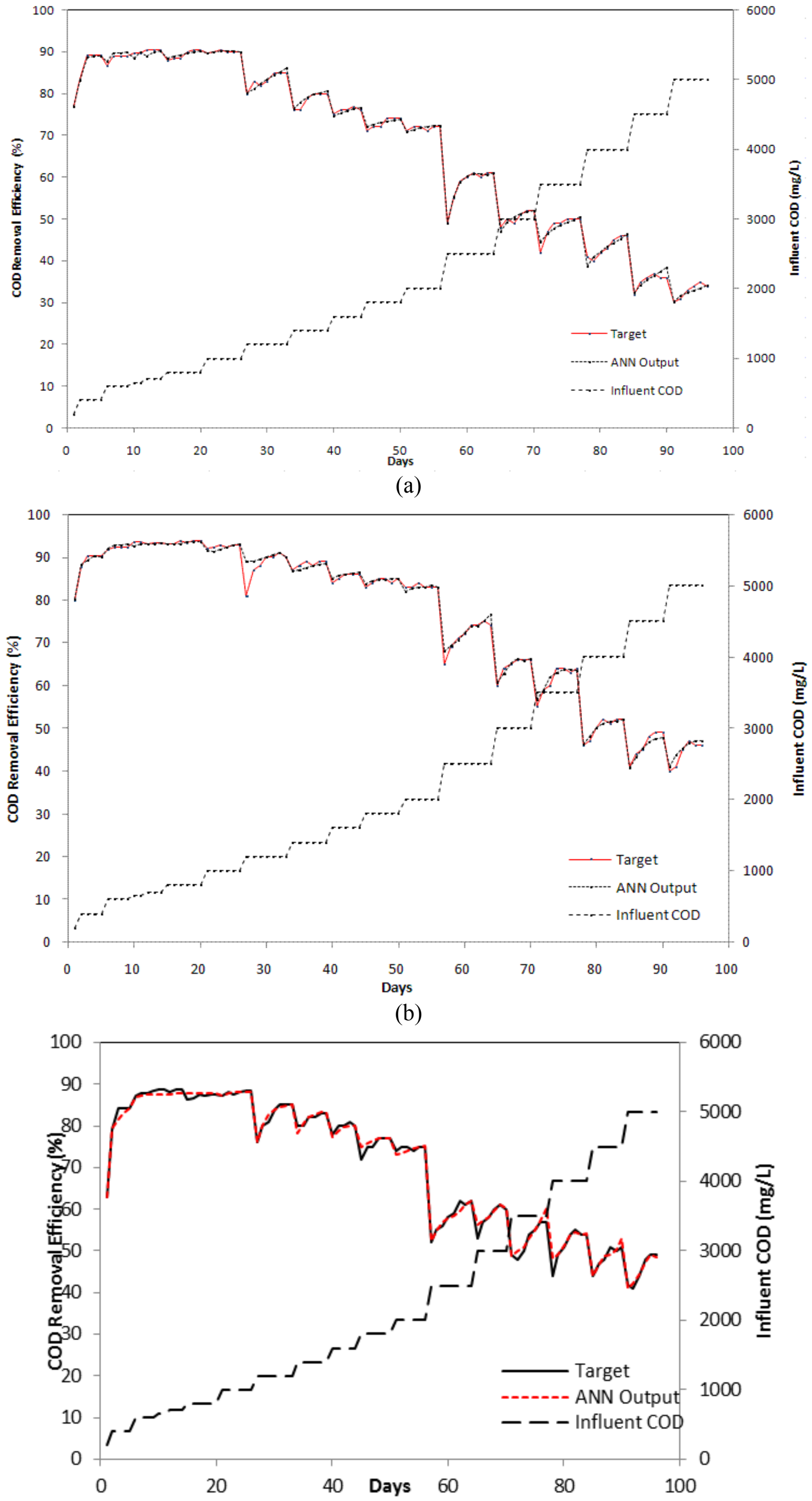


(c)

Fig. 5. Linear Regression between the network outputs and the corresponding training targets in the (a) first and (b) second stages of RBC with rotating discs and in (c) packed-cage RBC

Fig. 6 illustrates the performance of the optimized ANN models in predicting COD removal efficiencies of the RBC systems. For all three sets of the data, ANN models had a satisfactory accuracy in fitting the outputs and targets. So, it can be concluded that the proposed models are adequately able to predict the performance of both RBC with rotating disks and packed-cage systems.



(a) (b) (c)

Fig. 6. Performance of ANN model prediction in the (a) first and (b) second stages of RBC with rotating discs and (c) packed-cage RBC

4. CONCLUSION

In this study, a three-layer backpropagation neural network was optimized to predict the performance of rotating discs and packed-cage RBC systems in the degradation of hydroquinone (in terms of COD removal). The configuration of the backpropagation neural network which had the smallest MSE, was a four-layer ANN (3:6:6:1) with tangent sigmoid transfer function (tansig) with 6 neuron hidden layers. The output layer had linear transfer function (purelin), and Levenberg–Marquardt backpropagation training algorithm (LMA) had the best performance. Based on the findings of this study, the following conclusions can be drawn:

- Both RBC systems as advanced biological processes had proper COD removal efficiencies for treating hydoquinone synthetic wastewater. Up to 90, 93 and 88 percent removal efficiencies were obtained in RBC I, RBC II, and packed-cage respectively, for influent COD of 800 mg/L. The results of this study are comparable with similar research in recent years. For example, 90% removal efficiency of hydroquinone has been obtained for 700 mg/L influent COD using a MBBR [5]. In another study, with a bacterium (*Serratia marcescens AB90027*) as a catalyst, 96% of hydroquinone was removed in the influent COD of 3500 mg/L [3].
- During the experiments up to 4000 mg/L influent COD, RBC with rotating discs had higher removal efficiencies (about 5%-15%), but at higher loading rates, packed-cage RBC had better results.
- The model presents the ability of a feed-forward back-propagation neural network to predict the performance of RBC systems with a good accuracy. The model had a quite good performance in the estimation of not only the COD removal efficiencies used in training process, but also those of test data that were unfamiliar to the neural network.
- The designed, trained and validated artificial neural network model had a reasonable fit to the experimentally obtained data with a correlation coefficient (R^2) of 0.998 and 0.997 for RBC with rotating disks and packed-cage RBC, respectively.

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