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Prediction of Anoxic Sulfide Biooxidation Under Various HRTs Using Artificial Neural Networks

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Objective During present investigation the data of a laboratory-scale anoxic sulfide oxidizing (ASO) reactor were used in a neural network system to predict its performance. **Methods** Five uncorrelated components of the influent wastewater were used as the artificial neural network model input to predict the output of the effluent using back-propagation and general regression algorithms. The best prediction performance is achieved when the data are preprocessed using principal components analysis (PCA) before they are fed to a back propagated neural network. **Results** Within the range of experimental conditions tested, it was concluded that the ANN model gave predictable results for nitrite removal from wastewater through ASO process. The model did not predict the formation of sulfate to an acceptable manner. **Conclusion** Apart from experimentation, ANN model can help to simulate the results of such experiments in finding the best optimal choice for ASO based denitrification. Together with wastewater collection and the use of improved treatment systems and new technologies, better control of wastewater treatment plant (WTP) can lead to more effective maneuvers by its operators and, as a consequence, better effluent quality.

Key words: Artificial neural networks; Effluent sulfide prediction; Effluent nitrite prediction; Principal components analysis; Wastewater treatment; ASO reactor

INTRODUCTION

Our preliminary laboratory-scale studies have shown that anoxic sulfide oxidizing (ASO) reactor has been very efficient in biooxidation of sulfide utilizing nitrite as electron acceptor in synthetic wastewater. ASO reactor is an upflow bioreactor fed with synthetic wastewater containing sulfide and nitrite along with growth medium for microbial biomass. After a specified time period sulfide is converted to sulfate/elemental sulfur while nitrite is oxidized to dinitrogen. Microbial biomass contained in bioreactor is a mixture of various microbial populations collected from anaerobic digestion plant of Sibao Wastewater Treatment Plant (WTP) located in Hangzhou City, China. Being anoxic process, significant aeration cost savings is realized in ASO reactor for simultaneous removal of sulfide and nitrite. The potential achieved by decreasing HRT at fixed substrate concentration is higher than that by increasing substrate concentration at fixed HRT. The process can bear short HRT of 0.10 day but careful operation is needed. Nitrite conversion is more sensitive to HRT than sulfide conversion when HRT is decreased from 1.50 d to 0.08 d[1].

Improper operation of a WTP brings about serious environmental and social problems, as its effluents can cause or spread various diseases to human beings, as well as destabilize the natural environment where these wastes are disposed[2]. The water resources management is a highly complex issue covering a wide spectrum of activities in the field of assessment, planning, designing, operation, and maintenance. More effective maneuvers by its operators and better effluent quality can be achieved through combination of wastewater collection, the use of improved treatment systems and new technologies. A wide range of application of ANN

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and fuzzy logic techniques has been investigated in the field of water resources management.

Neural networks are very useful tools in pattern recognition because they allow classification without need for explicit recognition rules[3]. An artificial neural network (ANN) is a system that consists of a large number of simple processing units, called neurons as in the nervous system. A neuron generally has a high-dimensional input vector and a simple output signal. The function to be performed on the input vectors is hence defined by the non-linear function and the weight vector of the neuron. The strength of an ANN is that it trains itself and operates by a pattern of recognition of the data and arrives at a conclusion in an unbiased manner. ANN is traditionally used in the control researches, and in recent years, it has been successfully applied across a large range of domains, such as image recognition, medicine, molecular biology and, more recently, ecological and environmental sciences[4-5].

Hydraulic retention time (HRT) is the time a unit volume of wastewater will remain in anoxic sulfide oxidizing (ASO) reactor and overestimates the actual treatment time. At fixed substrate concentration with decreasing HRT determines the minimum time period for maximum treatment efficiency[1]. HRT may be one of the major factors causing variations in treatment efficiency. The effect of fluctuations in hydraulic and loading rates depends on the applied hydraulic retention time (HRT), sludge retention time (SRT), intensity and duration of the variations, sludge properties and the reactor design[6]. In view of fluctuations in ASO reactor removal efficiency encountered during performance tests, ANN based modeling is highly desirable for prediction of effluent quality under varying HRTs.

Aim of Study

There is no doubt that ANNs have great potential as tools for the prediction of water resources. The main purpose of this work was to predict the effluents of ASO process under different HRTs using neural networks in a wastewater treatment plant, aiming at predicting the plant parameters based on past information.

MATERIALS AND METHODS

Data Collection

Data used for present analysis was collected from a laboratory-scale ASO reactor operating for more than 130 days at Department of Environmental Engineering, Zhejiang University, China. Data were collected for various parameters such as influent and effluent sulfide, nitrite, nitrogen, sulfate, and pH values at different HRTs.

Artificial Neural Networks (ANNs)

In the early 1940s, McCulloch and Pitts[7] explored the competitive abilities of networks made up of theoretical mathematical models when applied to the operation of simple artificial neurons. The structure of an ANN defines the overall architecture of the network, including one input layer, one output layer, and usually one or two hidden layers (Fig. 1). Each neuron receives a weighted sum from each neuron in the preceding layer and provides an input to each neuron of the next layer. Thus,

$$net = \sum_{i=1}^{n} W_i X_i$$

Where *net* is the summation of the input signal, and W_i, denotes an element of the weight vector W, and X_i is an element of the input vector X. For a given network and input vector, the output vector is totally determined by the weights. The process of finding optimal weights is to find optimal weight, called "training". The training algorithms used in this study were back-propagation. The ANN parameters learning rate was 0.05, momentum constant 0.9, values

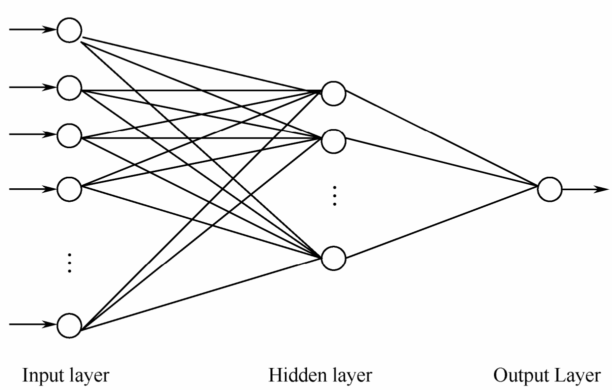

FIG. 1. Typical NN structure.

of MSE were 10^{-10} and activation function was Tan-sigmoid (Table 1). In this process, the input units and their desired output value were set for the network. The activations of the units were then calculated, feeding forward layer-by-layer from the inputs to the output. A logistic threshold function was used,

$$O = \frac{1}{1 + e^{-net}}$$

Where O is the output of the network. Once the network output value has been produced, it is compared with the target output specified in the training data set. Following this comparison, a backwards adjustment of the weights is performed and the training is stopped when the minimum error for test data found.

$$MSE = \frac{1}{n}\sum_{1}^{n}(P - O)^2$$

Where MSE is the mean square error considering prediction (P) and observed values (O) for n testing data vectors. The correlation coefficient (r) or determination coefficient (R^2) was used to evaluate the prediction. When r=1, there is a perfect positive linear correlation between P and O. When r=-1, there is a perfectly linear negative correlation between P and O. When r=0, there is no correlation between P and O. Intermediate values present partial correlation.

TABLE 1

ANN Influential Parameters Used During Training

Layer of Hidden Neurons	Activation Function	Learning Rate	Momentum Constant	Convergence Criterion	Epochs
1	Tan-sigmoid	0.05	0.9	$1e^{-10}$	2000

In our study, the input vector consists of 4 values (influent pH, sulfide, nitrite, and hydraulic residence time). The output value is a variable, such as sulfide, and N_2. The input data and output data were divided into training and testing data sets. The success of training was determined with the average sum square value between desired output vector and the predicted value, and the final error goal was set to 10^{-10}.

Statistical and Graphical Work

Statistical and graphical work was carried out using Sigma Plot v.10.

RESULTS

Influent Concentrations Selection

The data to perform artificial neural network analysis was obtained from anoxic sulfide oxidizing process utilizing sulfide as electron donor and nitrite as electron acceptor operated at various HRTs ranging from 2-0.8 d. Various inputs in ASO reactor, such as sulfide and nitrite, can result in the production of sulfate or sulfur (not measured), dinitrogen gas along with formation of some quantities of ammonium in the reactor. HRT along with pH can be regarded as important input variables in ANN analysis to predict the output. Thus four input variables (sulfide, nitrite, pH, and HRT) can result in the production of four outputs (sulfate, sulfur, nitrogen, and ammonium). The ranges of influent sulfide and nitrite used were 32-1920 mgS/L and 37.75-2265.25 mgN/L, respectively.

Network Selection

A neural network that uses gradient-descent error learning is designed and used in our prediction. The neural network has one input and one output. In the training of a BP neural network, 4 inputs (sulfide, nitrite, pH, and HRT) and one output vector sets are generated from the experiments. Experimental data from reactor operation of about 120 days are used as the learning set. The number of neurons in the hidden layer is generally selected from the different levels, such as one hidden layer (i.e. 4, 8, 12 layers) and two hidden layers (i.e. 25-12, 25-9, 12-8, 12-4), and 8 neurons in the hidden layer were found successful in the training process for experimental data. The training process has been completed approximately in 2000 iterations. When the training is completed, a neural network is designed using the obtained weights. In two-layered network, a 4-8-1 network is chosen and it can be successfully modeled for the current data.

The optimum performance of ASO reactor ranged for sulfide and nitrite influent concentrations of 32-1664 mgS/L and 37.75-1963.25 mgN/L, respectively, where sulfide and nitrite removal percentages were 99%-99.8% and 80%-94.47%, respectively. Based on optimization tests in ASO reactor, sulfide and nitrite concentrations of 1152 mg/L and 1359.25 mg/L respectively were selected for HRT tests. An optimum operation of a biological wastewater treatment plant (WTP) requires the effluent concentrations below the limits set by National Environmental Quality Standards (NEQS) or United States Environmental Protection Agency (USEPA). Though ASO process does not meet the demands of NEQS, it is very efficient in removing high sulfur and nitrogen loads. Moreover it can polish the effluents from secondary treatment.

ANN Prediction

The prediction of experimental data was conducted using the 8-1 ANN. Training data setting was based on the 50%-50% sampling technique. Initially, one-half of the cases were randomly selected and used with the BP network. Subsequently, the BP networks were trained for 2000 iterations. The root mean squared training error achieved by the networks is approximately 10^{-10}. Determining the training end point for the BP network is a tricky task. After training, the correlation coefficient between training and predictive values reaches 0.98 for field data and 0.99 for the training data, respectively. Changing the ANN influential parameters used during training increased the training time without any improvement in the model.

The relation between observed and predicted parameters during the performance of ASO reactor under various HRTs is presented in Figs. 2-6. Table 2 shows regression analysis for prediction of various parameters through ANN. As shown in Figs. 2-6, when the predicted values calculated by ANN were compared with the observed values, strong and positive correlation coefficients reached 0.88, 0.82, and 0.98 for pH, nitrite, and nitrogen, respectively. The model is very suitable to predict the effluent pH, nitrite, and nitrogen (Figs. 2-5). However, this model is weaker in predicting the effluent sulfide and sulfate (r=0.2 and 0.5) as shown in Table 2 and Figs. 3 and 6.

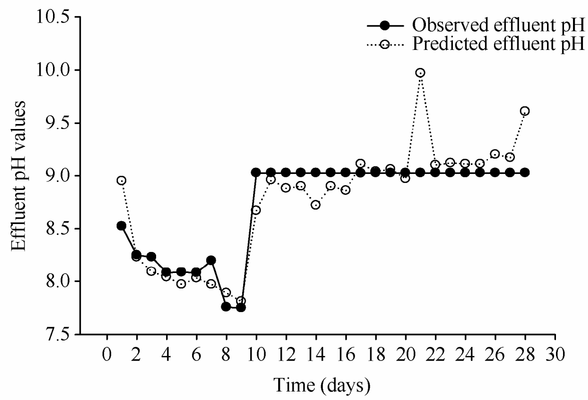

FIG. 2. Relation between observed and predicted effluent pH during HRT tests.

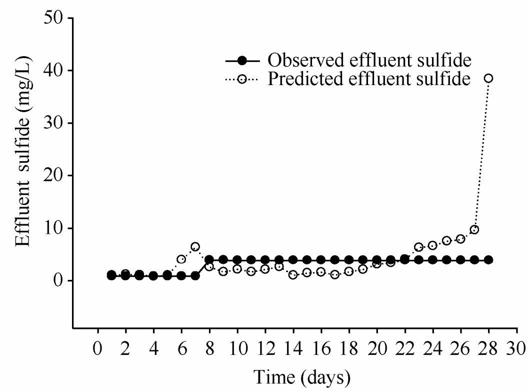

FIG. 3. Relation between observed and predicted effluent sulfide concentrations for HRT test.

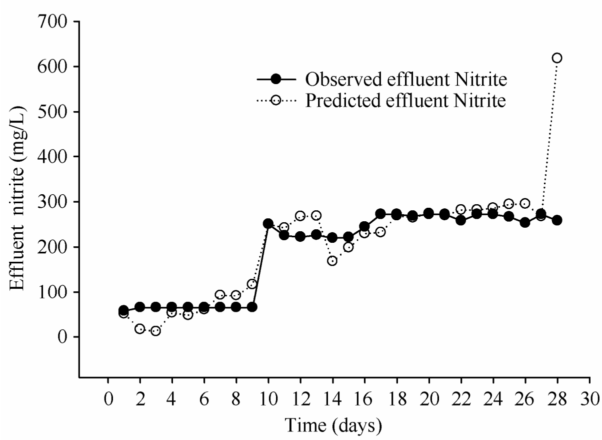

FIG. 4. Relation between observed and predicted effluent nitrite concentrations for HRT test.

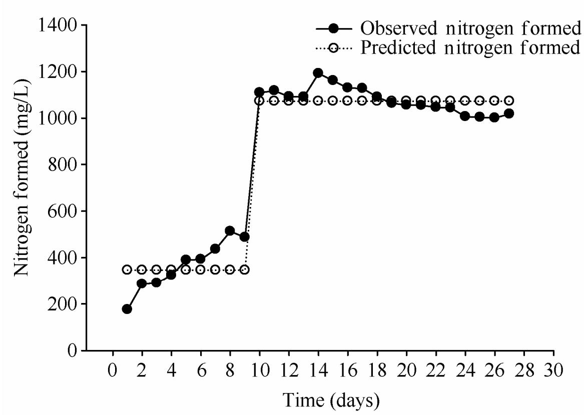

FIG. 5. Relation between observed and predicted nitrogen formed during HRT test.

TABLE 2

Non Linear Regression Analysis for Prediction of Various Parameters Through ANN

Statistical Parameters	pH	Sulfide	Sulfate	Nitrite	Nitrogen
r	0.88	0.20	0.58	0.82	0.98
RSqr	0.77	0.30	0.33	0.68	0.95

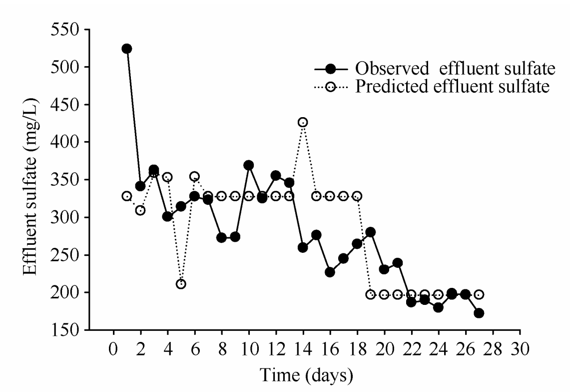

FIG. 6. Relation between observed and predicted effluent sulfate during HRT tests.

DISCUSSIONS

The present study showed that ANNs were able to model and predict effluents of anoxic sulfide oxidizing process based on the influent data. Present approach provides quite satisfactory prediction of effluent pH, nitrite and nitrogen for ASO reactor. However, the model cannot predict the formation of sulfide and sulfate for ASO process. Such unpredictable behavior of ANN model for sulfate is not surprising as there were many fluctuations in sulfate formation during actual experiment (Fig. 6). The actual experiment with ASO reactor at varying HRTs showed that nitrite removal was sensitive to HRTs fluctuations; however, ANN model could predict nitrite removal satisfactorily. So the model can be accepted based on the nitrite removal prediction. The rates of biochemical processes are governed by rules formally analogous to the rules valid for pure chemical processes. However, reaction rates of individual biochemical subprocesses are nonlinearly dependent on the plant state and environmental variables, such as temperature and pH. Frequently the dependence is nonmonotonic; some processes take place only in a narrow band of concentrations[8].

Applications of neural networks have rapidly increased recently. It has been shown that this technology is suitable for controling problems, making possible to achieve a better performance than those obtained by conventional models. The modeling traditionally used in bioprocesses is based on balance equations together with rate equations for microbial growth, substratum consumption and formation of products, and since microbial reactions coupled with environmental interactions are nonlinear, time-variable and of a complex nature[9-10], traditional deterministic and empirical modeling has shown some limitations[9,11]. Recently, some studies using artificial neural networks (ANNs) in modeling biological wastewater treatment processes have been published, providing an alternative approach[9-16]. This approach is potentially very efficient in obtaining more accurate predictions of process dynamics by combining a mechanistic and a non-parametric model either in parallel or in serial configuration in such a way that the non-parametric model properly accounts for unknown and non-linear parts of the mechanistic model. There has been a great preference in ANN, especially feed-forward back propagation neural networks (FBNN), as non-parametric model; however, the approach is applicable to other non-parametric models.

CONCLUSIONS

The future of anoxic sulfide oxidizing process seems bright. Based on the prominent results obtained during our preliminary laboratory-scale experiments coupled with more strict environmental regulations, ASO-based denitrification should be considered for simultaneous removal of sulfur and nitrogen from waste streams. The present study can be concluded as follows:

1. Within the range of experimental conditions tested, the ANN model gives predictable results for nitrite removal from wastewater through ASO process. The model does not predict the formation of sulfate to an acceptable manner.

2. Apart from experimentation, ANN model helps to simulate the results of such experiments in finding the best optimal choice for ASO based denitrification.

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