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Development of a Neural Network Technique for Prediction of Water Quality Parameters in the Delaware River, Pennsylvania

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Abstract: In the present study, artificial neural networks (ANN) were used to derive and to develop models for prediction the monthly values of dissolved oxygen and specific conductance as two water quality parameters of Delaware River at a station located at Pennsylvania site of the U.S. by using the monthly values of the other existing water quality parameters as input variables. The monthly data of four water quality parameters and discharge, for the time period 1995-2006 were selected for this analysis. In developing the ANN model for prediction of dissolved oxygen (DO) and specific conductance (SC), configuration 4-5-1 and 4-6-1 yielded optimal with 5 and 6 neurons in hidden layer respectively. Performance of the model was evaluated by statistical criteria includes correlation coefficient (r), root mean square error (RMSE) and mean absolute error (MAE). The correlation coefficients of ANN model for prediction of DO and SC were 0.980 and 0.989, respectively. Thus, a trained ANN model may potentially provide simulated values for desired locations at which measured data are unavailable yet required for water quality models.

Key words: Artificial neural network · Water quality parameters · Delaware River · Prediction · DO · SC

INTRODUCTION

Water quality is one of the main characteristics of a river, even when its purpose is other than human water supply. Therefore, assessment of the quality of surface waters is important in hydro-environmental management [1]. The surface water quality in a region largely depends on the nature and extent of the industrial, agricultural and other anthropogenic activities in the catchments. Human beings take water from the hydrologic cycle for their vital and economic needs and give it to the same cycle after using it [2]. Deterioration of water quality has initiated serious management efforts in many countries. Most acceptable ecological and water related decisions are difficult to make without careful modeling, prediction and analysis of river water quality for typical development scenarios [3].

Recent trends in the management of water supply have increased the need for modeling techniques that can provide reliable, efficient and accurate representation of the nonlinear dynamics of water quality within water distribution systems. Also, prediction of water quality parameters is one of the methods which have been recently considered for management of water resources. Water quality prediction enables a manager to choose an option that satisfies a large number of identified conditions. The predictions can be used for water resources planning and management in case they are of acceptable accuracy [4].

The river systems are most adversely affected due to their dynamic nature and an easy accessibility for the waste disposal directly or indirectly through drains/tributaries. Since, the rivers and streams are among most important sources of water for irrigation, industrial and other uses, these serve as the lifelines of the population staying in the basins. In general, the organic pollution in an aquatic system is measured and expressed in terms of the biochemical oxygen demand (BOD) and declined dissolved oxygen (DO) level. The DO level is measure of the health of the aquatic system and a certain

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level is essentially required for the aquatic life to survive [5]. Measures of DO refer to the amount of oxygen contained in water and defined the living conditions for oxygen-requiring (aerobic) aquatic organisms. DO concentrations reflect an aquilibrium between oxygen producing processes (e.g. photosynthesis) and oxygen consuming processes (e.g. aerobic respiration, nitrification and chemical oxidation) and the rate of atmosphere exchange. DO concentration in water column is maybe influenced by many factors such as temperature, pH and other water quality variables. Thus, it's important to develop predictive DO model for the management of water quality [6].

One of the other variables that indicate the quality of water is specific conductance. Specific conductance (SC) has been widely used as a measure of mineral salt concentration in both natural waters and soil solutions. Specific conductance is a measure of the ability of water to conduct an electrical current. It is highly dependent on the amount of dissolved solids (such as salt) in the water. Pure water, such as distilled water, has very low specific conductance, while sea water has high specific conductance. Specific conductance is an important water quality measure because it gives a good indication of the amount of dissolved material in the water. Like DO, it seems to be important to use a method for modeling this parameter. Therefore, both these parameters (DO and SC) are generally needed to be determined simultaneously and there is a need to devise some suitable secondary (indirect) method for predicting these variables in a large number of samples for water quality assessment.

In recent years, several researches have been conducted on water quality forecast models [7-9]. However, since a large number of factors affecting the water quality have a complicated non-linear relation with the variables; traditional data processing methods are no longer good enough for solving the problem [10].

In recent decades, numerical models have become indispensable tools for studying water quality parameters, contaminant transport and water resources management. On the other hand, new approach such as Artificial Intelligence techniques has proven their ability and applicability for simulating and modeling various phenomena in the water engineering field. In addition, artificial neural network (ANN) captures the embedded spatial and unsteady behavior in the investigated problem using its architecture and nonlinearity nature compared with the other classical modeling techniques [11]. The ANN, as its name implies, is a technique for the human brain's problem solving process. Just as humans apply knowledge gained from experience to new problems or situations, the structure of a neural network can be applied to powerful computation of complex nonlinear relationships [12].

Despite its strong theoretical potential, ANN application is subject to a number of challenges. In particular, it is widely recognized that the generalization of an ANN is dependent upon network topology and the selection of key network parameters, including the transfer function, the error function, learning rate and momentum [13]. A trial and error approach is often implemented to optimize ANN models, which can be extremely time consuming. Two types of automated techniques are available to select network architecture: pruning algorithms and constructive algorithms [14]. However, the specification of additional network parameters associated with such techniques limits their practicality.

ANNs have been successfully applied in a number of diverse fields, including water resources [15]. A multi-layer neural network can approximate any smooth, measurable function between input and output vectors by selecting a suitable set of connecting weights and transfer functions [3].

During last about two decades, ANNs have undergone an explosive development in application in almost all the areas of research [16- 24]. ANN models have been widely applied to the water quality problems [25-30]. This ultimately allows ANNs to model environmental systems without prior specification of the algebraic relationships between variables [28]. This has led to the application of ANNs in many water resources applications [31-36].

Chau (2006) has reviewed the development and current progress of the integration of artificial intelligence into water quality modeling [37]. Hatzikos *et al*., (2005) utilized neural networks with active neurons as a modeling tool for the prediction of seawater quality indicators like water temperature, pH, DO and turbidity [38]. Palani *et al*., (2008) demonstrated the application of ANNs to model the values of selected seawater quality variables, having the dynamic and complex processes hidden in the monitored data itself [39].

This paper presents the ANN model developed to predict DO and SC based on monthly measured water quality data at the Pennsylvania station of Delaware River (Fig. 1). The choice of input variables for the neural network modeling is based on a statistical correlation analysis and the availability of the field data too. The purpose of this study is to determine the extent to which

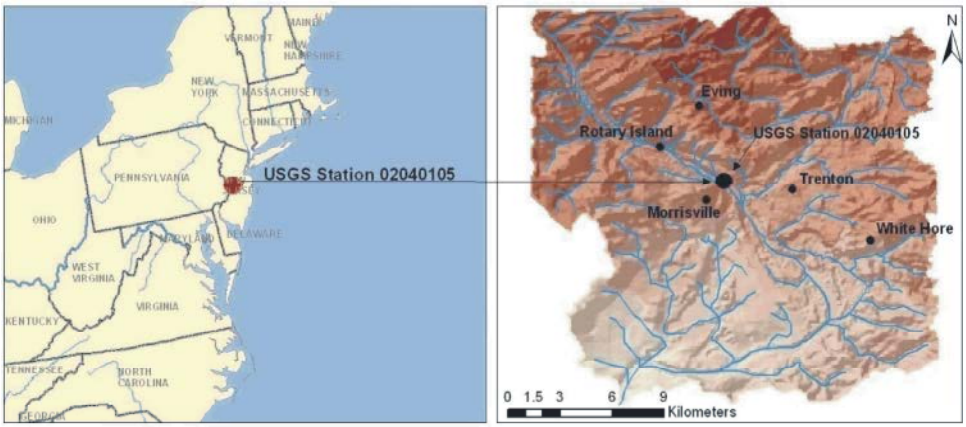

Fig. 1: The location of the Delaware River, Pennsylvania

Table 1: Water quality properties in the ANN model domain measured between July 1995and March 2006 in the Pennsylvania station

Parameters	Unit	Min	Max	Mean	SD
Temperature	°C	0.87	28.1	13.2	8.8
pH	-	6.9	8.9	7.9	0.37
Discharge	$ft^3.sec^{-1}$	2720	44020	13089	8876
DO	$mg.lit^{-1}$	7.5	15.3	11.2	2.2
SC	µS/cm	97.4	251.9	186.6	35.6

the DO concentration and SC in Delaware River can be predicted using continuous monthly measurements of selected water quality variables such as pH, temperature and discharge. Here, we have investigated the possibility of training ANN model correlating the primary water quality variables (independent variables) with their secondary attribute (dependent variable). The DO and SC of the river water were taken as the dependent variables here and set of other parameters constituted the independent variables.

Study Area and Water Quality Data: The water quality data of the stations operated by the U.S. Geological Survey (USGS) were used in the study. This investigation focuses on predicting DO and SC in the Delaware River at the Pennsylvania station (USGS station 02040105). This station is in the western part of Delaware State. Delaware is located on the eastern coast touching on the Atlantic Ocean. It is bordered by Maryland and there is a short border with Pennsylvania, New Jersey is across the Delaware Bay and Delaware River. Many small rivers flow across the state, some flowing New Jersey to the Delaware. The land is low-lying, from sand dunes in the south to rolling hills on the Pennsylvania border in the north. Delaware is quite flat, from sea level at the ocean beaches to an elevation of 442 feet above sea level in New Castle County. Chief agricultural products are broiler chickens, soybeans, corn and dairy products. Potatoes and other vegetables are also grown. Delaware has a moderate climate with an average monthly temperature ranging from 32 degrees Fahrenheit in the winter to 75.8 degrees Fahrenheit in the summer. The average annual precipitation is about 45 inches. This station located at 74° 46' 41" W and 40° 13' 18" N and has 20.65 ft elevation from mean sea level. The location of this station is illustrated in Fig. 1. For this station, the data from July 1995 to November 2002 were chosen for calibration and data from December 2002 to March 2006 were chosen for test (validation), arbitrarily.

The concentration range of the water quality variables measured between July 1995 and March 2006 in the Pennsylvania in the model domain is given in Table 1. In this table, SD indicates the standard deviation of any variable.

MATERIALS AND METHODS

Basic Principles of the Neural Networks: ANN models are highly flexible function-approximators that have shown their utility in a broad range of water resources applications [40, 41]. Most of these studies showed that ANNs performed better than classical modeling methods. The choice of the type of network depends on the nature of the problem to be solved. At the present time, the back-propagation multi-layer perceptron (MLP) is very popular and is used more than other neural network types

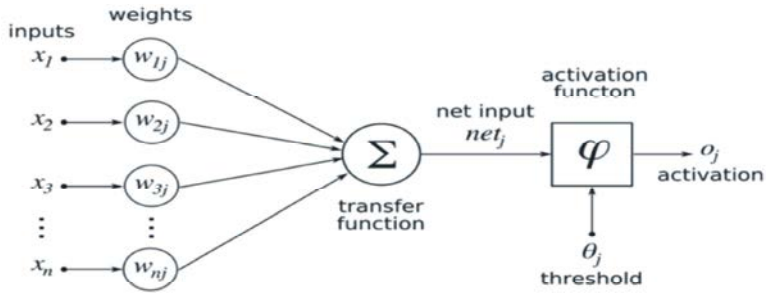

Fig. 2: The architecture of a back-propagation MLP

Fig. 3: Node j of a back-propagation MLP

for a wide variety of tasks. The back-propagation MLP is based on the supervised procedure; i.e., the network constructs a model based on examples of data with known outputs.

The architecture of the back-propagation MLP is a layered feed-forward neural network, in which the non-linear elements (neurons) are arranged in successive layers and the information flows uni-directionally, from input layer to output layer, through the hidden layer(s). As can be seen in Fig. 2, nodes from one layer are connected to all nodes in the adjacent layer(s), but neither lateral connections within any layer, nor feed-back connections are possible [29].

In this research, we assume that the back-propagation MLP uses the logistic function as its activation function. The net input $\hat{x}$ of a node is defined as the weighted sum of the incoming signals plus a bias term. For instance, the net input and output of node *j* in Fig. 3 are:

$$\bar{x}_j = \sum_i w_{ij} x_i + w_j, \tag{1}$$

$$x_j = f(\bar{x}_j) = \frac{1}{1+\exp(-\bar{x}_j)}, \tag{2}$$

where x_i is the output of node *i* located in any one of the previous layers, w_{ij} the weight associated with the link connecting nodes *i* and *j* and w_j the bias of node *j*. Since the weights w_{ij} are actually internal parameters associated with each node *j*, changing the weights of a node will alter the behavior of the node and in turn alter the behavior of the whole back-propagation MLP. First, a squared error measure for the *p*th input–output pair is defined as:

$$E_p = \sum_k (d_k - x_k)^2 \tag{3}$$

where d_k is the desired output for node k and x_k is the actual output for node k when the input part of the *p*th data pair is presented. To find the gradient vector, an error term ε_j for node j is defined as:

$$\varepsilon_j = \frac{\partial E_p}{\partial \bar{x}_j} = \frac{\partial \sum_k (d_k - x_k)^2}{\partial \bar{x}_j} \tag{4}$$

By the chain rule, the recursive formula for ε_j can be written as:

$$\varepsilon_j = \begin{cases} -2(d_j - x_j)\dfrac{\partial x_j}{\partial \bar{x}_j} = -2(d_j - x_j)x_j(1-x_j), \text{If node j is an output node,} \\ \dfrac{\partial x_j}{\partial \bar{x}_j}\sum_{k,j\le k}\dfrac{\partial E_p}{\partial \bar{x}_k}\dfrac{\partial x_j}{\partial x_j} = x_j(1-x_j)\sum_{k,j\le k}\varepsilon_k w_{jk}, \text{Otherwise,} \end{cases} \tag{5}$$

where w_{jk} is the connection weight from node *j* to *k* and w_{jk} is zero if there is no direct connection. Then the weight update Δw_{jk} for off-line learning is:

$$\Delta w_{jk} = -\eta \frac{\partial E}{\partial w_{jk}} = -\eta \sum_p \frac{\partial E}{\partial w_{jk}} \tag{6}$$

where η is a learning rate that affects the convergence speed and stability of the weights during learning. In vector form,

$$\Delta w = -\eta \Delta_w E \tag{7}$$

where

$$E = \sum_p E_p \tag{8}$$

This corresponds to a way of using the true gradient direction based on the entire data set. The way we adapt to speed-up training is to use the momentum term:

$$\Delta w = -\eta \nabla_w E + \alpha \Delta w_{prev} \quad (9)$$

where w_{prev} is the previous update amount and the momentum constant a, in practice, is usually set to something between 0.1 and 1. As for the detail of the back-propagation MLP, interested readers can refer to any books addressing neural network theory for more information [28].

An ANN software package, Qnet2000, is adopted herein the study. The requirements of the neural computation algorithm are such that raw data are usually normalized to an interval by transformation. The transformations modify the distribution of the input variables so that it matches the distribution of the estimated outputs. In this study, before the training of the network both input and output variables were normalized within the range 0.1-0.9 as follows:

$$x_i = 0.8\frac{(x - x_{\min})}{(x_{\max} - x_{\min})} + 0.1 \quad (10)$$

where x_i is the normalized value of a certain parameter, x is the measured value for this parameter, x_{min} and x_{max} are the minimum and maximum values in the database for this parameter, respectively.

Training: The training process determines the ANN weights and is similar to the calibration of a mathematical model. The ANNs are trained with a training set of input and known output data. At the beginning of training, the weights are initialized either with a set of random values, or based on some previous experience. The goal of learning is to determine a set of weights that will minimize the error function (Garson, 1991). As training proceeds, the weights are systematically updated according to a training rule. Several training examples are presented to the network and the process is terminated when the difference between measured and estimated value is less than a specified value. At this stage, the ANN is considered trained.

The network is trained to produce an estimated output vector when $\hat{Y}(n)$ presented with an input pattern $X(n)$. The error function at the n^{th} input exemplar, $E(n)$ is given by:

$$E(n) = \frac{1}{2}\left(\hat{Y}(n) - Y(n)\right)^2, \quad (11)$$

where $\hat{Y}(n)$ is the estimated state of the output unit in response to the nth input exemplar and $Y(n)$ is the desired state of the output unit. After the (n+1)th input exemplar is presented, the weight is generally update by:

$$\Delta w_{ji}(n+1) = -\eta \frac{\partial E}{\partial w_{ji}} - \xi \Delta w_{ji}(n) \quad (12)$$

where η represents the learning rate, which for practical purposes, is chosen as high as possible without causing the oscillation of the convergence of the network. ζ is a constant (momentum term) that determines the effect of past weight changes on the current weight change.

Evaluation of Performance: A model trained on the training set can be evaluated by comparing its predictions to the measured values in the overfitting test set. These values are calibrated by systematically adjusting various model parameters. The performances of the models are evaluated using the root mean square error (RMSE) [Eq. (13)], the mean absolute error (MAE) [Eq. (14)] and the correlation coefficient (r) [Eq. (15)]. Scatter plots and time series plots are used for visual comparison of the observed and predicted values. R^2 values of zero, one and negative indicate that the observed mean is as good a predictor as the model, a perfect fit and a better predictor than the model, respectively. Depending on sensitivity of water quality parameters and the mismatch between the forecasted water quality variable and that measured, an expert can decide whether the predictability of the ANN model is accurate enough to make important decisions regarding data usage.

$$RMSE = \left[\sum_{p=i}^{N}\left(d_p - x_p\right)^2 / N\right]^{1//2} \quad (13)$$

$$MAE = \frac{1}{N}\sum_{p=1}^{N}\left|d_p - x_p\right| \quad (14)$$

$$r = \frac{N\sum_{p=1}^{N} d_p x_p - (\sum_{p=1}^{N} d_p)(\sum_{p=1}^{N} x_p)}{\sqrt{[N\sum_{p=1}^{N} d_p^2 - (\sum_{p=1}^{N} d_p)^2] \times [N\sum_{p=1}^{N} x_p^2 - (\sum_{p=1}^{N} x_p)^2]}} \quad (15)$$

where d_p is the desired (target) value, x_p the ANN output for the pth pattern and N the total number of patterns.

RESULTS AND DISCUSSION

Different ANN models were constructed and tested in order to determine the optimum number of nodes in the hidden layer and transfer functions. Selection of an appropriate number of nodes in the hidden layer is very

important aspect as a larger number of these may result in over-fitting, while a smaller number of nodes may not capture the information adequately. Fletcher and Goss (1993) suggested that the appropriate number of nodes in a hidden layer ranges from ($2n^{1/2}$+m) to (2n + 1), where n is the number of input nodes and m is the number of output nodes. Subsequently, two different ANN models were constructed for the computation of DO and SC in the river water. The network was trained using the training data set and then it was validated with the validation data set. This network is designed by putting weights between neurons, by using the hyperbolic-tangent function of training [42]:

$$f(s) = \tanh(s) = \frac{e^{s} - e^{-s}}{e^{s} - e^{-s}} = \frac{1 - e^{-2s}}{1 + e^{-2s}} \quad (16)$$

where $s_i = \sum_{i=1}^{n} w_i x_i$, in which w_i weights and x_i are input values.

For neural network models construction, monthly data partitioned training (70% of all data) and tests (the remaining 30% of all data) data sets, were used. For the ANN models construction for the both water quality parameters (DO and SC) chosen to be used as output, two other water quality parameters (Temperature and pH) and discharge (Q) considered as inputs.

In the present study, the following combinations of input data of flow were evaluated:

- pH and Temperature
- pH and Discharge
- Temperature and Discharge
- pH, Temperature and Discharge

The output layer had 1 neuron for DO or SC. The configuration giving the minimum RMSE and maximum correlation was selected for each of the combinations. Table 2 gives the correlation and RMSE for each combination for DO model. It is clear from Table 2 that the ANN model whose inputs are pH, Temperature and Discharge (input combination 4) performs better than the other ANN models.

Several MLP networks were generated and tested for the input combination 4. Back-propagation algorithm (BPA) was used to adjust the learning procedure. We used momentum and weight decay to improve the network. The results of different MLP and their errors for DO are shown in Table 3. These results are derived from three rows of unlearned data. Mean absolute percentage error (MAPE) for each model is calculated from the following equation:

$$MAPE = \frac{1}{N} \sum_{i=1}^{N} \frac{\left| x_p - d_p \right|}{d_p} \quad (17)$$

where d_p is the desired (target) value, x_p is the ANN output for the pth pattern and N is the total number of patterns.

In the trials, the number of neurons in the hidden layer varied between 4 and 7. As can be seen from Table 3, the model 3 outperforms the others. The optimal SC model was also obtained using same manner.

The optimal combination with the better prediction results for each of two variables used as outputs are given in Table 4.

As seen from Table 2, the architecture of the optimal ANN model for the DO model is composed of one input layer with three input variables, one hidden layer with five nodes and one output layer with one output variable. The correlation coefficient (r), RMSE and MAE values computed for the training and test data sets are presented in Table 2. Fig. 4 shows the plot between measured and computed DO values by ANN in training and validation sets. The selected ANN (3 nodes in input layer, 5 nodes in hidden layer and single node in output layer) provided a best fit model for all the two data sets. A closely followed pattern of variation by the measured and model computed DO concentrations in river water (Fig. 2), r, RMSE and MAE values suggest for a good-fit of the DO model to the data set.

SC is another associated with major water quality parameters due to the dilution effect of stream flow, so that it can be used as a general water quality indicator. Significant changes in conductivity could then be an indicator that a discharge or some other source of pollution has entered a stream. In case of the SC, the ANN model was developed to simulate and predict the SC at Delaware River, USA. Both DO and SC used an ANN architecture back propagation for this station with a hidden layer with hyperbolic-tangent transfer function.

The selected ANN (three nodes each in input and seven nodes in hidden layers and single node in output layer) provided a best fit model for all the two (training and test) data sets. Fig. 5 shows the plots between the measured and computed values of SC by ANN in training and validation sets.

The scatter plots of actual versus predicted values of DO and SC obtained using ANN model are shown in Fig. 6a-b, respectively. The figure reveals that an acceptable agreement between the simulations and observations can be achieved. The correlation coefficient values between the ANN models predicted values and observed data for dissolved oxygen and specific

Table 2: RMSE and coefficient of correlation for ANN model-training and testing data

	Training data		Validation data	
	DO (mg/lit)		DO (mg/lit)	
ANN model input	Correlation	RMSE	Correlation	RMSE
pH and Temperature	0.978	0.355	0.971	0.565
pH and Discharge	0.984	0.339	0.980	0.538
Temperature and Discharge	0.982	0.344	0.981	0.534
pH, Temperature and Discharge	0.986	0.330	0.980	0.531

Table 3: Different MLP results for DO

MLP model number	1	2	3	4	5	6
Number of neurons in first hidden layer	4	5	5	6	6	7
Number of neurons in second hidden layer	2	1	0	2	0	2
Relative error (MAPE)	0.052	0.036	0.031	0.043	0.048	0.064

Table 4: Performance parameters of the ANN models for computation of the DO and SC in the Delaware River water (Pennsylvania station).

Model	ANN-structure	Data set	RMSE	MAE	r
DO	3-5-1	Training	0.33	0.26	0.986
		Validation	0.53	0.37	0.980
SC	3-7-1	Training	4.74	2.05	0.990
		Validation	6.21	2.44	0.989

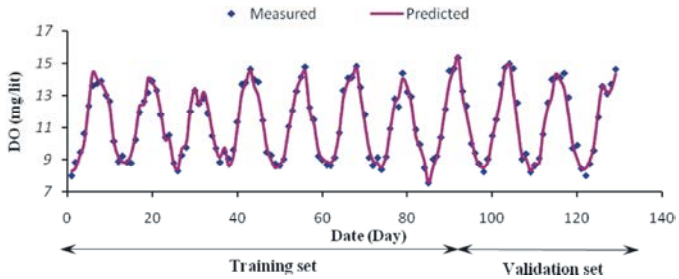

Fig. 4: Comparison of the predicted and measured DO levels in the river water for training and validation sets using ANN model

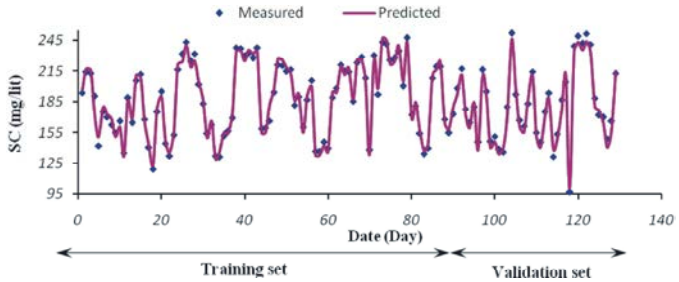

Fig. 5: Comparison of the predicted and measured SC levels in the river water for training and validation sets using ANN model

conductance are 0.980 and 0.989, respectively, which are satisfactory in common model applications. These results indicate that the neural network model is able to recognize the pattern of the water quality parameters to provide good predictions of the monthly variations of water quality data (DO and SC) of the Delaware River.

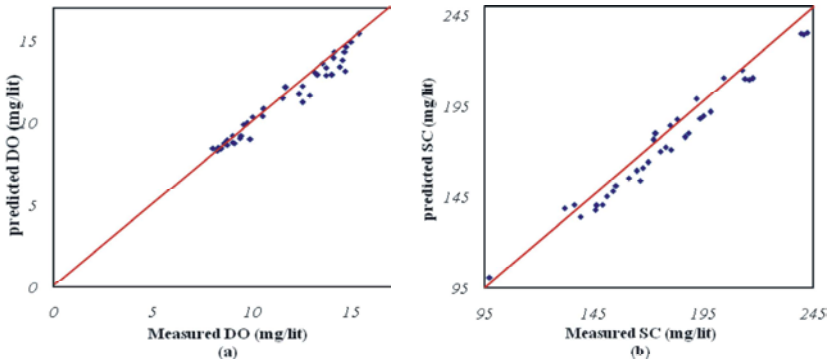

Fig. 6: Scatter plots of actual versus predicted DO values (a) and SC values (b) for the test data set obtained using ANN model

Generally, Table 4 and Figures 4, 5 and 6 clearly demonstrate the ability of the neural network models to predict very well the monthly values of the DO and SC at the Pennsylvania station.

CONCLUSIONS

This manuscript recommends the use of ANN-based water quality parameters prediction model for rivers. In this paper, artificial neural network models were developed for prediction the monthly values of two water quality parameters DO and SC in the Delaware River, Pennsylvania. The monthly data of these and three other water quality variables, pH, temperature and discharge (Q), at Pennsylvania station, for the time period July 1995 and March 2006 were selected for this analysis. The networks were designed by putting weights between neurons, by using the hyperbolic-tangent function of training. The results for the training and the test data sets were satisfactory. Hence, with the proposed model applications it is possible to manage water quality parameters such as DO and SC in a more cost-effective and easier way. Consequently, it has been demonstrated that DO and SC in the Delaware River can be predicted with acceptable accuracy from a small set of physical and meteorological measurements.

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