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Predicting Atmospheric Concentrations of Benzene in the Southeast of Tehran using Artificial Neural Network

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ABSTRACT

Air pollution is a challenging issue in some of the large cities in developing countries. In this regard, data interpretation is one of the most important parts of air quality management. Several methods exist to analyze air quality; among these, we applied the Multilayer Perceptron (MLP) and Radial Basis Function (RBF) methods to predict the hourly air concentration of benzene in 14 districts in the municipality of Tehran. Input data were hourly temperature, wind speed and relative humidity. Both methods determined reliable results. However, the RBF neural network performance was much closer to observed benzene data than the MLP neural network. The correlation determination resulted in 0.868 for MLP and 0.907 for RBF, while the Index of Agreement (IA) was 0.889 for MLP and 0.937 for RBF. The sensitivity analysis related to the MLP neural network indicated that the temperature had the greatest effect on prediction of benzene in comparison with the wind speed and humidity in the study area. The temperature was the most significant factor in benzene production because benzene is a volatile liquid.

Key words: Tehran, MLP neural network, RBF neural network, Benzene, Air pollution

1. INTRODUCTION

Air pollution in urban areas is a challenging problem, especially in the developing world. The increasing number of vehicles and the existence of a large number of older cars in the cities has worsened air pollution. Several air pollution parameters exist, such as particulate matter and carbon monoxide ozone. Benzene has been selected in our research because this chemical threatens public health. Benzene, a colorless liquid with a pleasant odor, is a volatile compound. Exposure to benzene with a concentration of 20,000 parts per million (ppm) for a period of between 5 to 10 minutes can be fatal (International Agency for Research on Cancer, 1988) and it causes cancer diseases (Cruz-Núñez *et al*., 2003; Jo and Song, 2001). The results of the studies describe how exposure to benzene causes acutenonlymphocytic leukemia and preleukemia (Cruz-Núñez *et al*. 2003; WHO, 1989). The exposure limit of benzene in the workplace is 0.5 ppm, according to suggestions from the Occupational Safety and Health Ministry (USA) (Maltoni *et al*., 1990). Therefore, benzene in the air can be a public health problem and needs to be studied. Availability of air pollution data can help air quality management plan a reduction pollution program. Several methods exist to interpret the data, such as deterministic and probabilistic techniques. Among them, the ANN neural network is the most popular one used to analyze air quality parameters.

Many researchers have applied the artificial neural network (ANN) method to predict air pollution, such as Ruiz-Suárez *et al*. (1995); Tasadduq *et al*. (2002), Owega *et al*. (2006), Sousa *et al*. (2007), Sadr Mosavi and Rahimi (2008), Kurt *et al*. (2008), Bodaghpour (2008), Moustris *et al*. (2010), Bodaghpor *et al*. (2011), Chattopadhay and Chattopadhay (2012), Moustris *et al*. (2013).

Other researchers compared the results by ANN-based methods with those by a time series, multiple linear regression or principle component analyses, and they concluded that the ANN models successfully worked for the prediction of air pollution better than the other models mentioned above (Noori *et al.,* 2013; Sousa *et al.,* 2006; Grivas and Chaloulakou, 2006). In addition, Charkhastani and Bodaghpour (2008) and Al-Alawi *et al*. (2008) reported that the combination of the ANN with a principle component regression method further reduced the error between observed and predicted atmospheric concentrations of air pollutants.

Building deterministic models requires several parameters which were not available in our study. As mentioned previously, several researchers proved the ANN results are superior to time series, regression analysis and principal component. The ANN is able to simulate many of the complicated nonlinear processes (Manhaj, 1998). For predicting air quality, it is necessary to have a day's or a week's worth of data in advance. The MLP and RBF can predict the future value. Therefore, we applied MLP and RBF to our data.

The first objective of our work was to apply the MLP and the RBF neural network to predict benzene concentration in the air in the southeast of Tehran. The second purpose was to determine which parameters, including temperature, humidity and wind speed, were significant in benzene prediction.

The study area is located in the southeast of Tehran and the geographic coordinates of the city are 51°, 2′ and, 51°, 36′ East longitude and 35°, 34′ and 35°50′ North latitude. The elevations of Tehran are 2000, 1200 and 1050 meters in the north, in the center and in the south, respectively. The north and east of the city is surrounded by the Alborz Mountains and the main source of precipitation is the Mediterranean. The Alborz Mountains and Atlantic winds that blow from the West act as a barrier to prevent the penetration of air masses. Tehran is also located in an arid and semi-arid region. The temperature variations are between 40 Celsius in summer and -5 Celsius in winter. The annual rainfall is about 250 millimeters. Fig. 1 shows the study area.

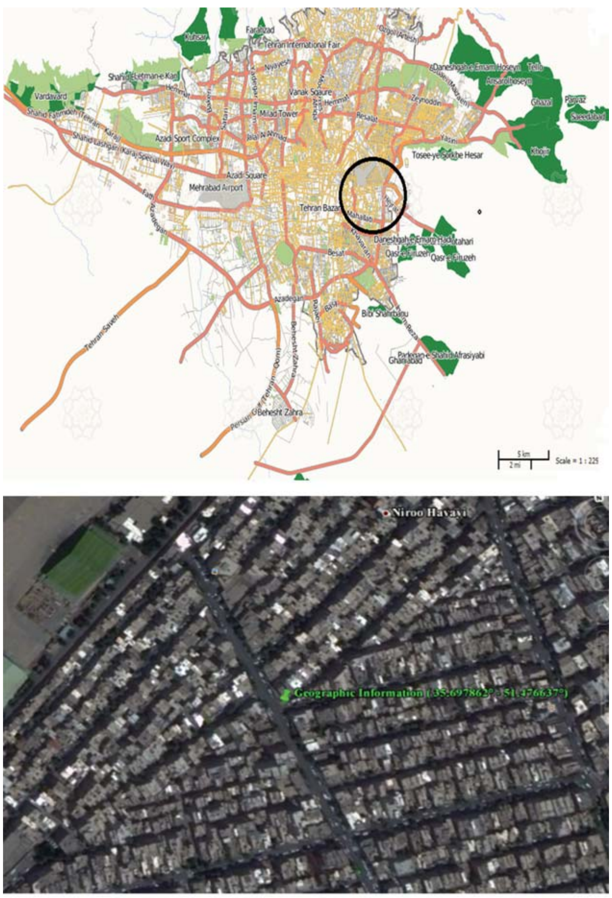

Fig. 1. The location of the study area with graphical information.

2. EXPERIMENTAL METHOD, MATERIAL

Considering the availability or the preparation of accurate and sufficient data for training, the ANN is very important and the power of the ANN for responding to the new problem depends on the primary data to some extent. Therefore, sufficient and precise data is necessary to train the network well until the network can extend or predict data for the future propose. The air quality parameters were the hourly temperature, wind speed, humidity and benzene. Nine hundred and forty eight pieces of data was available, from which 800 were applied for training the network and the rest of them for comparing the simulation data with observed data. The data were monitored by the Air Quality Control Company (AQCC) of the municipality of Tehran. The AQQC collected data during late July through late September 2010. The availability of the data was the limitation in our study. However, the amount of data was sufficient for our work. The study area was district 14 of the municipality of Tehran (southeast of Tehran).

The artificial neural network (ANN) is a data processing system, based on a model of the human neurological system that consists of three unique components, including weighting (W), bias (B) and the transfer function (f). Output is computed by the Equation 1:

$$a=f(n)=f(wp+b) \tag{1}$$

Where "p" and "n" are input and output, while "a" is net input and f is transfer function. The input layer works as an interface between the input variable data and the ANN model. Most models also contain one or two hidden layers although more are possible. These layers implement most of the iterative calculations

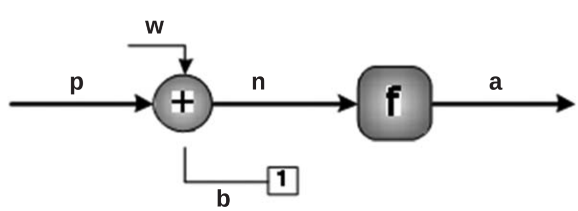

Fig. 2. Schematic of artificial neural.

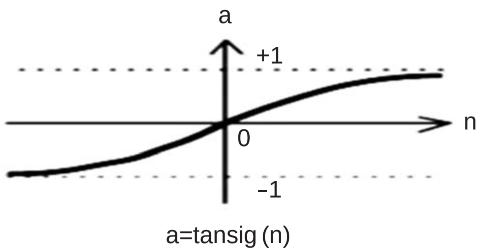

Fig. 3. Transfer function tangent sigmoid.

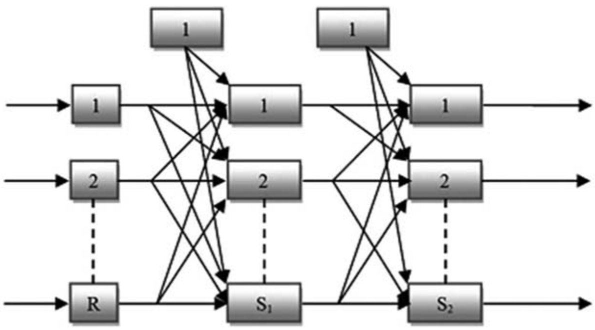

Fig. 4. The MLP with a hidden layer (asadollahfardi *et al.*, 2012).

within the network. The output layer serves as the interface between the ANN model and the end user, transforming model information into an ANN-predicted value of the output variable. Several types of transfer functions exist. Among them We applied the tangent sigmoid function (Fig. 3), which creates output in the range of (-1,1) and introduces non-linearity into the network, which can capture non-linear relationships between input and output values. Static and dynamic neural networks are two types of artificial neuron network. We applied both Multi-Layer Perceptron (MLP) and Radial Basis Function (RBF). Consequently, the static type outputs of the network at any time depend on the inputs at the same time, which means time independence (Menhajans and Safpour, 1998).

2.1 The MLP Neural Network

The MLP is a static type of the ANN (Fig. 4). The number of neural neurons in the hidden layers for each model can be calculated by trial and error. The MLP with a hidden layer, tangent sigmoid transfer function and linear layer outputs can be modeled by equations 2 and 3 (Menhaj, 1998).

$$a_j^1(t)=F\left[\sum_{i=1}^{R} w_{i,j}^1\, p_i(t)+b_j^1\right] 1\le j\le S_1 \quad (2)$$

$$a_k^2(t)=G\left[\sum_{j=1}^{S_1} w_{k,j}^2\, a_j^1(t)+b_k^2\right] 1\le k\le S_2 \quad (3)$$

Where R is the number of input vector components, S_1 and S_2 are numbers of neural in hidden and output layers, respectively. P is input vector. w_1, w_2 are weighting matrix in hidden and output layers, respectively. b_1, b_2 are bias vectors in hidden and output layers, respectively. G and F are transfer functions in hidden and output layers.

2.2 Determination of Network Architecture

To determine a suitable number of hidden layers in the ANN and its relationship with an optimal performance of the network is always a point of discussion. If the selected number of hidden layers is low; it is likely that the mapping is not properly estimated. Conversely, too many hidden layers increase the network intricacy. Furthermore, augmenting the number of layers does not necessarily lead to an increase in network accuracy. Hornik *et al.* (1989) confirmed the "universal approximator theory" which explained that a feed forward neural network with a hidden layer of sigmoid tangent and linear output layer can estimate each complicated function (Leshno *et al.*, 1993; Hornik, 1993, 1991; Cybenko, 1989). This theory reduces the number of hidden layers in the least amount and declines the complexity of the network (Hornik *et al.*, 1989). The rate of the network efficiency depends on using a suitable number of neural in hidden layers. However, in our study, we applied the ANN with one and two hidden layers. The transfer function of the hidden layer is a sigmoid tangent and the function of the output layer is considered a linear tangent. We developed a program and defined it in the Matlab software (2012) to select the numbers of neurons in two hidden layers and then to calculate the number of their errors. Afterward, we selected the neuron numbers which contained minimum errors.

2.3 Learning Rate

A parameter is the named learning rate in the training algorithm of back propagation, which is on the basis of the steepest descent. Its aim is to minimize the sum square error of outputs. Obtaining the suitable learning rate is one of the most sensitive processes of applying the algorithm of back propagation. The learning rate is described by a symbol α and determines the velocity of convergence in this algorithm. The performance of the steepest descent algorithm is enhanced if the learning rate is allowed to change during the training process. An adaptive learning rate attempts to make the learning step as big as possible to keep the learning stable and requires some changes in the training procedure.

The sigmoid functions are applied in the MLP and characterized by the fact that their slopes must approach zero as the input gets larger. This causes a problem when steepest descent is applied to train a multilayer network with sigmoid functions, since the gradient can have a very small magnitude; consequently, it can potentially cause small changes in the W and B, although the W and B are far from their optimal values. Resilient back propagation training algorithm is used to eliminate these harmful effects of the magnitudes of the partial derivatives (Asadollahfardi *et al.*, 2012).

2.4 Data Preparation

Upon considering using a tangent sigmoid of the transfer function in the hidden layer of the networks, we changed the scale of the data. All applied data, output and input were transformed to the -1 and 1 interval to prevent network saturation. After finishing the process, the predicted values were transformed back to the real data. We applied Equation 4 to change the scale of the data (Razavi, 2006).

$$A_s=\frac{O_t-A}{B-A}\times 2-1 \tag{4}$$

Where A_s and O_t are scaled and the observed value of the benzene, temperature, humidity and wind speed at time t, respectively. A and B is the lowest and highest amount of a series of the parameters.

2.5 Evaluation of Models

To determine the amount of error in predicting of benzene and performance evaluation of the models, we applied Volume Error (VE), Mean Absolute Error (MAE), a Root Mean Squared Error (RMSE) and Mean Bias Error (MBE) which are indicated in Equations 5 through 8.

$$VE=\frac{1}{n}\sum_{t=1}^{n}\left|\frac{O_t-F_t}{O_t}\right|\times 100 \tag{5}$$

$$MAE=\frac{1}{n}\sum_{t=1}^{n}|O_t-F_t| \tag{6}$$

$$RMSE=\sqrt{\frac{1}{n}\sum_{t=1}^{n}(O_t-F_t)^2} \tag{7}$$

$$MBE=\frac{1}{n}\sum_{t=1}^{n}\left|\frac{F_t-A_t}{A_t}\right| \tag{8}$$

Where F_t and O_t are the predicted and the observed values of BOD at time t, respectively, and n is the number of data.

Also, we applied the Index of Agreement (IA) and coefficient of determination (R^2) between observation and predicted data to illustrate the validity of the model (Eqs. 9 and 10) (Heckman, 1979).

$$IA=d=1.0-\frac{\sum_{t=1}^{N}(A_t-F_t)^2}{\sum_{t=1}^{N}(|F_t-\bar{A})+|A_t-\bar{A})|^2} \tag{9}$$

Where, A_t, F_t and $\bar{A}$ are observed (recorded) data, predicted data and mean observed data, respectively (Willmott *et al.*, 2012).

$$R=\frac{\sum(O-\bar{O})(F-\bar{F})}{\sqrt{\sum(O-\bar{O})^2\sum(F-\bar{F})^2}} \tag{10}$$

Where, O and F are observed and predicted data, respectively. $\bar{O}$ and $\bar{F}$ are the average of O and F, respectively (Kennedy, 1964).

2.6 The Radial Basis Function (RBF)

While the structure of the RBF is identical to the MLP, the RBF simulates the unknown air quality using a network of Gaussian basis functions in the hidden layer (Equation 9) and linear activation functions in the output layer (Dawson and Wibly, 2001).

$$f(x)=e^{-x^2}/_{2\sigma^2} \tag{11}$$

Where x is the weighted sum of inputs to the neuron, σ is the sphere of influence or the width of the basis function, and f(x) is the matching output of the neuron (Dawson and Wibly, 2001):

The RBF neural networks consist of a very simple architecture. Their structure contains an input layer, a single hidden layer, and an output layer, which, at each output node, makes available a linear combination of the outputs of the hidden-layer nodes. Training an RBF includes two steps. First, the basic functions are computed using an algorithm to cluster data in the training set. Kohohen self-organizing maps (SOMs) or a *k*-means clustering algorithm is most often used. Kohohen SOMs (Kohohen, 1984) are a form of 'self-organizing' neural network that learn to differentiate patterns within input data. Therefore, a SOM will, consequently, cluster input data according to perceived patterns without containing a corresponding output response. *K* means clustering and includes the organization of all objects into a predefined number of groups by minimizing the total squared Euclidean distance for each object with respect to its nearest cluster center. Other techniques such as orthogonal least squares and Maxi Min algorithms have also been applied (Song, 1996). Subsequently, the weights linking the hidden and the output layer are computed directly applying the simple matrix inversion and multiplication. The direct calculation of weights in an RBF makes it faster in training in comparison with an equivalent MLP (Dawson and Wibly, 2001).

3. RESULTS

The statistical summary of the data is presented in Table 1.

Table 1. The Statistical summary of the data used in this study.

Data	Benzene $10^{-6}\frac{g}{m^3}$	Temperature C°	Wind velocity m/s	Relative humidity %
Average	5.52	31	2.42	23
Peak	33.46	36	9.8	29
Minimum	1.22	23	0.3	12
Count	948	948	948	948

As illustrated in Fig. 5, we trained the ANN network using input parameters which were temperature, wind speed and humidity. The Root Mean Squared Error (RSME) decreased as iteration was increasing. However, the number of errors was relatively unchanged after 10 iteration numbers (epoch). Therefore, we stopped the train of the network at 10 iteration numbers. In each epoch, input parameter data were introduced to the network and it created an output parameter which was benzene. Afterward, the error of the network was calculated. Finally, the parameters of the ANN network were amended according to the number of errors. Fig. 5 describes training, validation and testing errors of the MLP neural network for different iterations.

Tables 2 and 3 indicates some of the neuron results together with their errors in one and two hidden layers

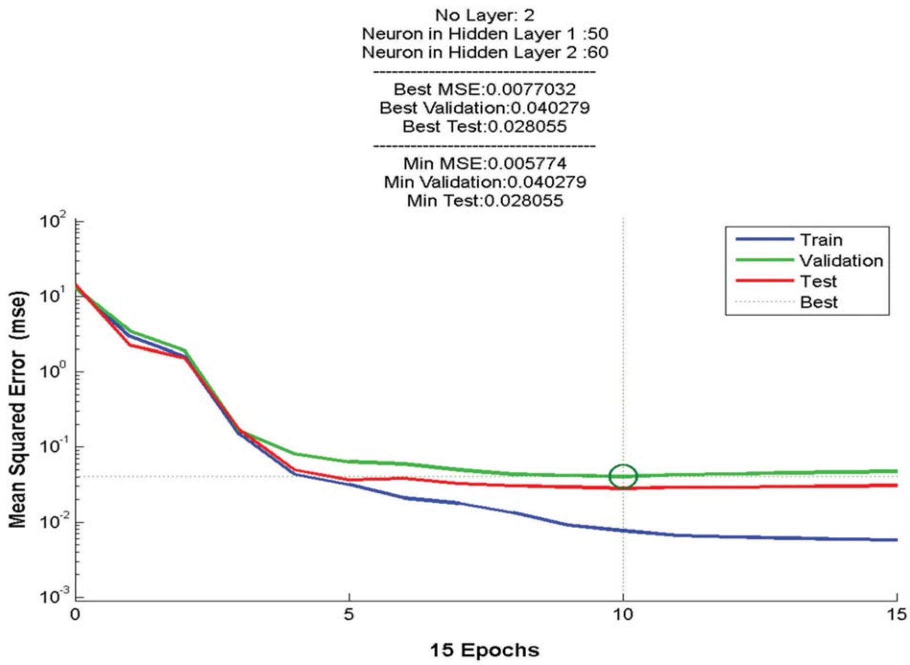

Fig. 5. Training, validation and testing errors of the MLP for different iterations.

Table 2. The error values for the MLP network with a hidden layer and different neurons in testing stage.

Neuron number	VE error	MAE error	RMSE error	Neuron number	VE error	MAE error	RMSE error
1	88.32	2.76	3.05	110	38.88	1.83	2.01
5	77.16	2.42	2.67	120	32.3	1.72	1.08
10	84.92	2.62	2.9	130	37.8	1.2	1.31
40	42.27	1.33	1.47	140	35.1	1.1	1.22
50	62.4	1.95	2.15	**155**	**25.4**	**0.805**	**0.89**
60	45.85	1.43	1.58	160	26.35	0.82	0.93
70	41.06	1.28	1.41	170	25.52	0.84	0.98
80	35.5	1.11	1.23	180	28.7	1.05	1.11
90	34.4	1.05	1.19	190	26.33	0.83	1.02
100	58.79	1.22	1.35	200	27.2	0.87	1.15

Table 3. The testing error values for the MLP network with two hidden layers and different neurons.

Neuron number	VE error	MAE error	RMSE error
2-2	80.84	2.55	2.81
2-5	76.08	2.4	2.64
2-12	71.92	2.27	2.5
2-21	79.84	2.51	2.77
2-25	64.23	2.05	2.28
50-50	30.92	0.98	1.1
50-55	27.74	0.87	0.96
51-55	45.59	1.33	1.47
50-60	**20.81**	**0.66**	**0.73**
53-54	38.82	1.22	1.34
53-56	30.51	0.96	1.06
53-57	49.15	1.56	1.72

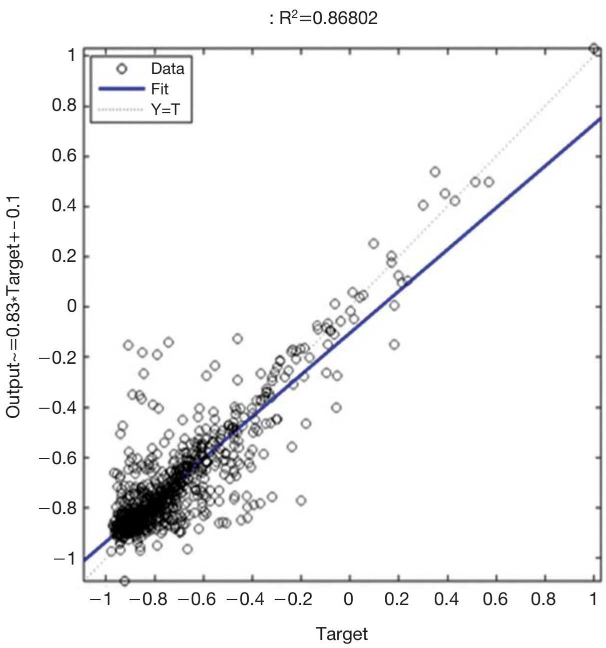

Fig. 6. The normal plot between observed and predicted benzene data of the MLP network (testing).

in the MLP neural network. As indicated in Table 3, the number of errors in testing of two hidden layers is less than a hidden layer in the MLP. Therefore, we selected the MLP neural network with two hidden layers.

We selected two hidden layers containing 50 and 60 neurons in the first and second layer since it contained a minimum error for the MLP neural network and the Mean Bias Error was 0.209. The MSE error was 0.007 (Fig. 5). Fig. 6 indicates the normal plot of selecting the proper network. The coefficient of determination between observed and predicted data was 0.868 and the Index of Agreement (IA) was 0.889, which indicates the accuracy of the model. The horizontal axis of Fig. 6 is observed value and vertical axis are predicted value.

Fig. 7 also illustrates a comparison between the observed and the predicted benzene data. As indicated in the figure, relatively good agreement exists between the two types of data.

We selected 800 neurons in the hidden layers as a starting point to train the network and the RBF neural network to decrease the number of neurons with iteration to reach a neuron which had a minimum error. As depicted in Fig. 8, in the training process of the RBF network, when iteration numbers (epoch) increase, the errors of the network decline. The training step stops in two situations. First, when the number of errors reaches zero. Second, when increasing the numbers of epochs, the number of errors does not change. In our work, the amount of error was about 0.1. Decreasing the number of errors, improves the performance of the model. The MBE was 0.131, which means the estimation of the model is acceptable.

The aim of the training process was to reach zero errors and then the train was stopped. Fig. 8 also illustrates the training, validation and testing of the training of the network.

Fig. 9 presents the normal plot between observed and predicted benzene data of the RBF network. The coefficient of determination between observed and predicted benzene was 0.907 and the Index of Agreement (IA) was 0.937, which indicates the accuracy of the model, which in turn confirms the suitability of the RBF network. As previously mentioned, the horizontal axis of Fig. 9 is observed value and vertical axis is predicted value.

Fig. 10 also illustrates a comparison between observed and predicted benzene data of the RBF network. As depicted in the figure, a good agreements between two types of data exist.

The published studies associated with using artificial neural networks to predict benzene in the air were rare. Therefore, we could not compare the results of our work with similar studies. However, the result of our work indicates the RBF neural network prediction is much closer to the observed data than the MLP neural network, which is similar to the results of Sun *et al.* (2008) and Haiming and Xiaoxiao (2013). The results of the work may be applicable for short time prediction of benzene because of the duration of the data collection. Nevertheless, the amount of data for developing the models was adequate.

3.1 Sensitivity Analysis

For sensitivity analysis, we increased and decreased one of the input parameters and the rest of the parameter data remained unchanged. After that, the changed

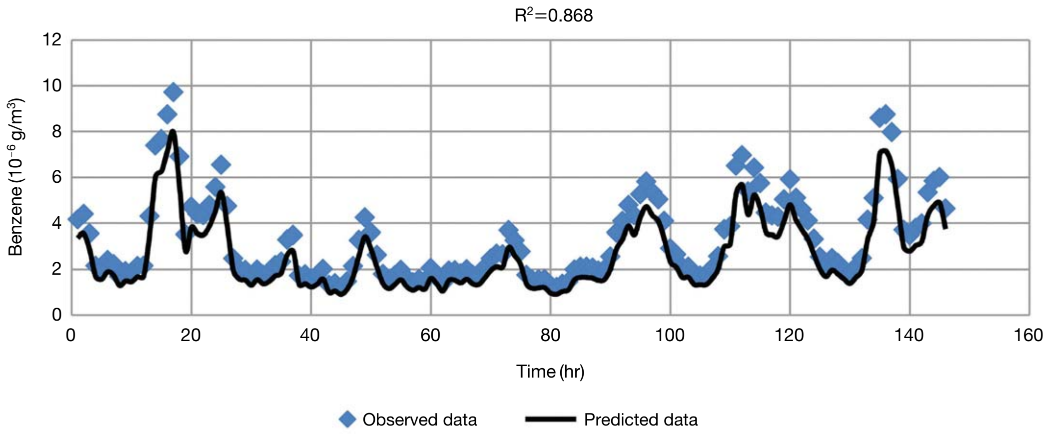

Fig. 7. A comparison between observed and predicted benzene data using the MLP network.

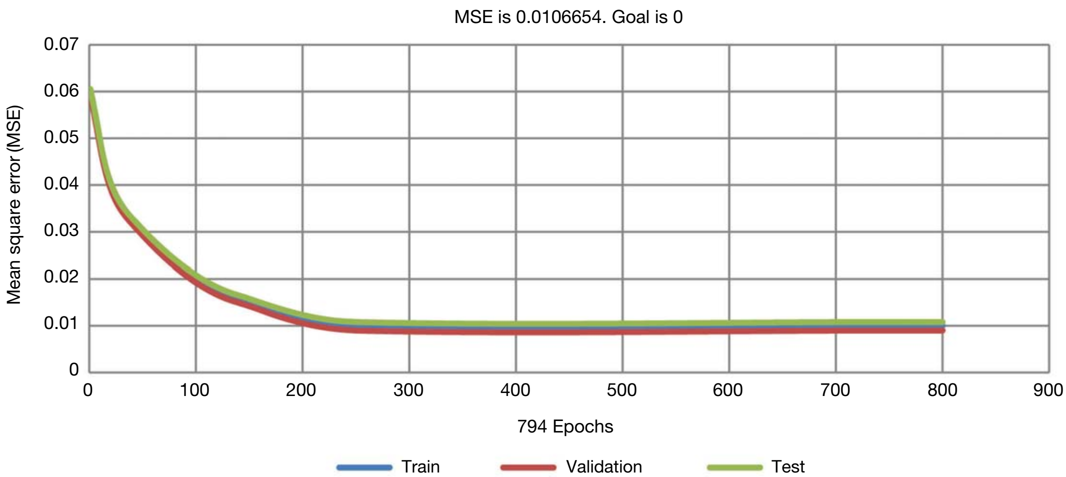

Fig. 8. The performance of the RBF network in reduction of RSME errors in the training process.

data and two other parameter data were used as a new input to the MLP neural network. Afterward, we determined the new coefficient of determination between new predictions and the observed data for benzene. We continued this procedure for the rest of the parameter data. Table 4 indicates the results of our sensitivity analysis. As illustrated in the table, temperature was the first factor affecting the predicting of benzene. Wind speed and humidity were the second and third factor in the prediction of the benzene, respectively. Temperature is the first factor because benzene is a volatile liquid.

Four types of petroleum losses occur in gas stations in Tehran, which include delivery losses, fill pipe emissions, breathing losses and seepage. While the underground storage tanks in gas stations are filled up with petroleum, existing air in the storage tank is forced to move into the atmosphere which contains a considerable amount of benzene. Fill pipe emission is the second factor for increasing the amount of benzene in the atmosphere. When cars are filled up, the air inside the tank is forced to move out of the tank and causes an increase of benzene in the atmosphere. The amount of existing petroleum steam in one cubic meter from the car's tank equals one cubic meter emitted from an underground storage tank in petroleum station (Wallace,

Table 4. The results of the Sensitivity analysis.

Parameters	R^2		
	Changing data		Not changing data
	+20%	−20%	
Temperature	0.72	0.75	0.868
Wind speed	0.81	0.72	0.868
Relative humidity	0.80	0.81	0.868

1990; Dean, 1985). The third factor, which is called breathing loss, occurs during the day from increasing temperatures. Two factors affect the emission of steam from petroleum. The first factor is steam emerging by simple thermal expansion of petroleum from underground storage tank and second, steam come from evaporation of petroleum caused by increasing air temperature (Wallace, 1990; Dean, 1985). Petroleum overflow from the car's tank and seepage from pumping stations are the fourth factor of lost petroleum which causes an increase in benzene.

Also, decreasing wind speed indicators affect the forecasting ability of the developed model in comparison to the increasing wind speed. Finally, relative humidity does not appear to play an important role in benzene prediction.

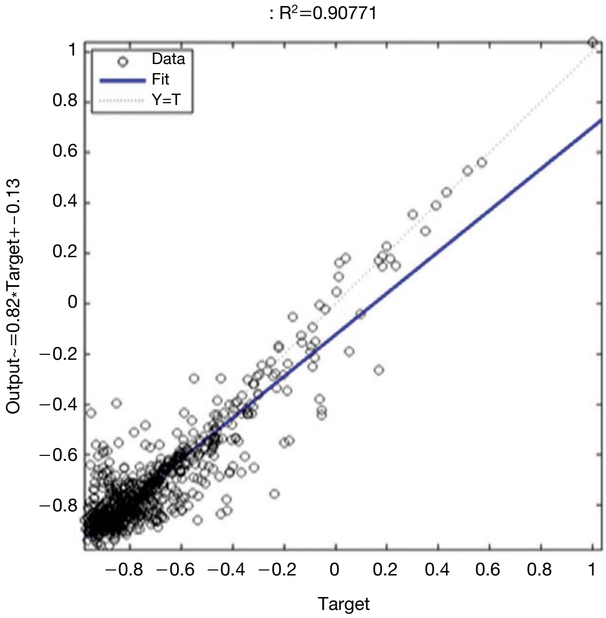

Fig. 9. The normal plot between observed and predicted benzene data of the RBF network (testing).

4. CONCLUSIONS

Taking into consideration the results and discussions of the MLP and the RBF neural network associated with the benzene pollution in the southwest of Tehran, we summarized the following conclusions:

1. The MLP neural network with two hidden layers including 50 neurons in the first layer and 60 neurons in the second layer contained a minimum error in testing. The MAE, VE and RMSE were 20.81, 0.66 and 0.73, respectively.
2. The RBF, with a hidden layer, contained a minimum error in training, validation and testing in comparison with the MLP neural network. The RMSE was 0.007.
3. The coefficient of determination between the observed and predicted benzene data for both MLP and RBF neural networks was 0.868 and 0.9077, respectively.
4. The results of the sensitivity analysis indicated that temperature, wind speed and humidity are the first, second and third factors affecting the prediction of benzene, respectively.
5. Comparison between the results of the MLP with the RBF neural networks in predicting benzene indicates that the forecasting of the RBF is closer

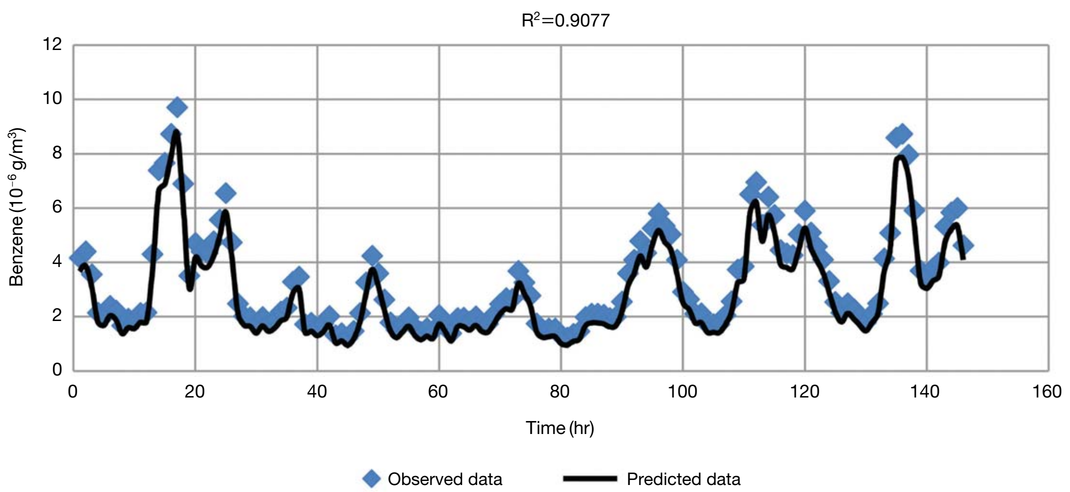

Fig. 10. Comparisons between observed data with the predicted data using the RBF neural network.

to observed data than the MLP neural network.

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