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THE SIMULATION OF THE IMPACT OF THE POLLUTION FACTORS ON THE PHYSICAL AND CHEMICAL PARAMETERS OF THE AIR QUALITY ALONG THE ROMANIAN COAST OF BLACK SEA USING NEURAL MODELS

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The aim of this research is to identify and investigate the pollution sources along the Romanian coast of the Black Sea, especially in the Constanta neighbourhood, by monitoring the air quality parameters. Furthermore, we will try to disseminate the information collected and we will propose adequate actions to prevent the continuous degradation of the environment. Several sampling sites were established around and inside the Constanta city resort, and analyses were carried out monthly. Physical and chemical parameters of the air quality, such as temperature, wind speed, Carbon Dioxide (CO_2), methane (CH_4), Nitrogen Oxide, ozone and water vapour concentrations are monitored "in situ" in different sampling sites of the Romanian Black Sea coast. The values of quality-monitored parameters are variable in quasi-large ranges, depending on the position of the sampling sites. A direct correlation between these indicators can be done. Air pollution causes the "greenhouse effect", and has a high impact on plant life and fauna, destroying the Black Sea ecosystems. The most important measures to remedy the area are the installation of more efficient filters in the industrial area, the cleaning of residual water, and the building of special places to collect the residues, to prevent direct discharge in the surface water. In our research we developed a neural simulation model of a wide database concerning the air pollution inside Constanta resort city, and based on this, to predict future results.

Keywords: Neural model simulation; neural networks; air pollution factors; prediction

1. Introduction

The atmosphere gases responsible for keeping a normal temperature on the planet are Carbon Dioxide (CO_2), methane (CH_4), Nitrogen Oxide, ozone and water vapours - all of

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these coming from natural sources. When the concentration of these gases increases, much more heat will be absorbed, and consequently the air temperature increases too.

In the last 100 years, the global temperature average increased by 0.6 [^{0}C], and in Europe by 1.2[^{0}C]. However the last 10 years were the warmest , with the exception of 1996. The weather forecast statistics reveal that by 2010 the temperature will increase by 1.4-5.8[^{0}C], and will be much more accentuated in the East and South-East side of Europe, including the Constanta zone. The global warmth magnitude could be kept under control only by reducing the emission of the "greenhouse effect" gases. Air is very important in nature, and its protection must be considered when thinking about the future of our planet. The air, like water, is one of the most crucial factors with a high impact to the quality of the life. Obviously the development of the maritime port and the industrial zone have an important impact on the local environment. During the last decade (2000-2010) we make reference to many international meetings and international conventions which have the stabilization of the "greenhouse effect" gas concentration in atmosphere as the main objective in order to prevent the dangerous disorder of the planet's climate system. Almost all of the international conventions are concerned with the diminution of SO_2 and NO_x emissions, produced by high capacity burn installations, and decreasing activity of petroleum chemistry and refinery plants. The "greenhouse effect" gas concentration could be decreased by a long term decrease of energy consumption, the identification of renewable energy resources, and an increase in energy efficiency. A rough estimation reveals that the cost of investment for decreasing the emissions is approximately 45 euro/person/year compared to 300-1500 euro/person/year otherwise. The current position of the EU is already well known, and it aims to reduce gas emissions by 20% by 2020, which could be increased to above 30% if other well developed countries such as the USA, China and India become much more involved, but the Copenhagen's Protocol from the end of 2009 was a big deception. The ambitious EU objective for 2020 is equivalent to the complete reduction of the gas emission from the transportation industry in all of Europe.

2. The air quality factors, the pollution and the "greenhouse gas effect" emission analyses

The atmosphere is a mixture of uncontaminated air, water vapours and different impurities. The natural impurities represent a small amount and can consist of: meteoric debris, natural powder particles, NaCl, NO_2, SO_2, HCl, H_2S, ozone, bacteria, pollen, powder, condensation nuclei, and impurities created by industrial activities. In the present research we analyse the level of the "greenhouse gas effect" emissions for Constanta resort city during 2006. Especially in this study we analyse the impact on the air quality of the following air pollution agents: CO, NH_3, N_2O, ozone, H_6C_6, and the debris. The maximum permissible emission of the pollution agent represents the pollution amount released into the atmosphere, without significant changes. It is represented by the pollution agent threshold. If the pollution agent exceeds its threshold then some precautions will need to be imposed, namely: close up the pollution sources, pollution agents cleaning, and the evacuation of people from the neighbourhood. This research was initiated based on the measurement data archive provided by the Environment Protection Agency from Constanta. An overall image of the levels of “greenhouse gas effect” emissions during 2000-2008 for the main pollution nutrients in Constanta city is given in Figures 1-3. The statistics from the Environment Protection Agency and the General Clinic Hospital from Constanta based on different data sets regarding the concentration of the pollution agents in air and their effects on the human healthy reveal very interesting results and at the same time attract the attention of the governmental authorities to be more responsible and more involved in reducing the short and long term damages as soon as possible. The effect of the pollution due to human activity is not observable immediately or in the short term. The pollution represents an accumulative process, invisible to the human eye and it could affect our future generations. Generally speaking, the diseases caused by the gas emission of different industrial activities will appear in time and become dangerous especially for the young and for old people. The common effect of the pollution due to gas emission is respiratory and cardio-vascular diseases.These statistics mainly use the correlation method to make the link between different diseases and the pollution agents that cause these diseases. The distributions of people with respiratory problems affected by the pollution are represented in Figure 4, both men and women, from both the rural and urban environment.

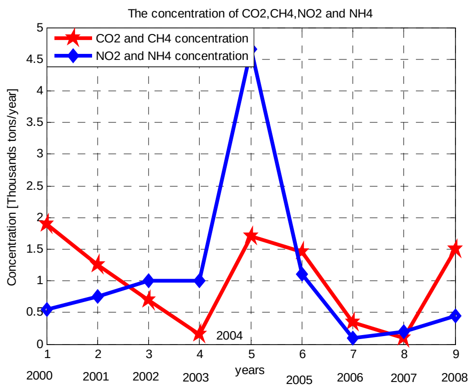

Fig.1. The evolution of the carbon dioxide (CO2), methane (CH4), Azote dioxide (NO2), and Ammonia (NH4) concentrations in the air during the period 2000-2008

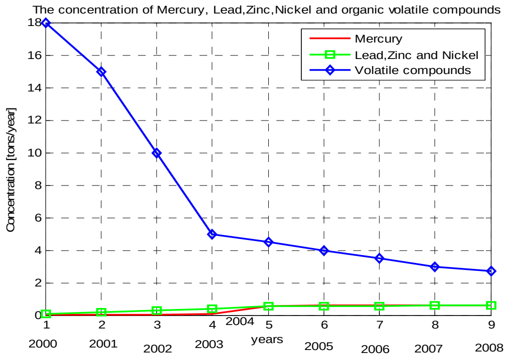

Fig.2.The evolution of the metals (H_g, P_b, Z_n, N_i) and volatile organic compounds concentration in the air during the period 2000-2008

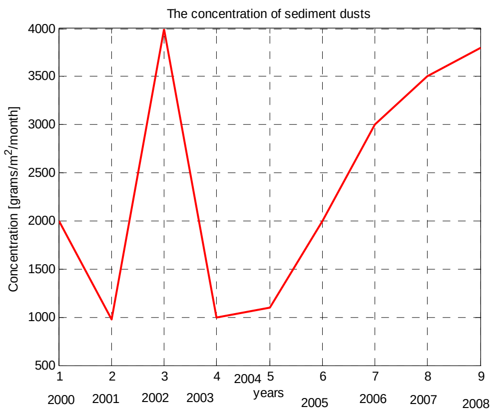

Fig.3.The evolution of the sediment dusts concentration in the air during the period 2000-2008

Fig.4.The distribution of people with respiratory problems by residency (urban, rural) and by gender

The measurement data set is represented by the monthly average based on 15 samples (daily average), expressed in mg/m^3. The maximum levels of the pollution agents are established using different standards, such as the well-known ISO and STAS 10331-75. In our study we use the measurement data set based on the samples taken during the reference year (2006). Inside the Constanta resort city the air quality is recorded “in situ” by seven automated samples stations located in representative sites. Our research is based only on the samples collected from the CET Constanta measurement station. The pollution agents recorded are those recognized by Romanian laws, based on the European standards. The limit values being imposed by OM 592/2002 are such that the precarious effects on people’s health and on the environment are prevented and reduced. The following meteorological parameters are also recorded: speed direction, pressure, temperature, solar radiation, relative humidity and rainfall. The concentrations of some of these air pollution agents during the reference year 2006 are presented in the Tables 1 and 2.

Table 1

Concentration of the chemical air pollution ingredients

Month	NO_2 [$\times 10^{-3}$ mg/m^3]				NH_3 [$\times 10^{-3}$ mg/m^3]				CO [$\times 10^{-3}$ mg/m^3]			
	Min	Avg	Max	Cmp	Min	Avg	Max	Cmp	Min	Avg	Max	Cmp
January	0,3	1.28	3.17	0,1	0	7.1	27.4	0,1	22	233	245	2
February	0,4	1.7	4.4	0,1	0,4	2.5	14	0,1	2.3	249	115	2
March	0	0.8	1.9	0,1	0	6.3	11.6	0,1	1.1	483	112	2
April	0,4	1.5	3.8	0,1	0,7	5.2	19	0,1	14	533	116	2
May	1	2	3.2	0,1	0	1.3	4.6	0,1	3	555	165	2
June	0,12	1.3	2.5	0,1	0	2.9	10	0,1	18	614	218	2
July	0,2	1.5	3.8	0,1	1.2	4.1	7.7	0,1	5	201	238	2
August	0,14	1.5	1.8	0,1	0,32	2.4	6.1	0,1	20	837	149	2
September	0,3	0.74	1.5	0,1	2	6	12	0,1	4	351	231	2
October	0,14	0.4	0,5	0,1	0	4	12	0,1	60	109	440	2
November	0,3	0.5	0,6	0,1	1.4	5.1	10.8	0,1	11	307	407	2
December	0,3	0.7	1.3	0,1	0	2.2	11.8	0,1	21	141	363	2

Table 2
Concentration of the chemical air pollution ingredients
*Min-minimum value, Avg-average value, Max-maximum value, Cmp-maximum permissible value

Month	$O_3[\times 10^{-3}$ mg/m$^3]$				C_6H_6 $[\times 10^{-3}$ mg/m$^3]$				Powders $PM_{10}[\times 10^{-3}$ mg/m$^3]$			
	Min	Avg	Max	Cmp	Min	Avg	Max	Cmp	Min	Avg	Max	Cmp
January	23	62.6	96	30	1.34	6.86	9.9	80	118	420	480	15
February	35	52.2	75	30	1.47	5.46	8.2	80	78	240	396	15
March	12	61.7	94	30	1.12	3.79	6.5	80	238	528	1025	15
April	9	24.7	76	30	3.56	5	7	80	81	308	658	15
May	29	30.1	85	30	1.16	6.1	8.7	80	83	385	753	15
June	8	42.2	68	30	1.10	6.8	12.3	80	72	219	1333	15
July	9	33.1	79	30	1.28	8.13	21.7	80	80	344	743	15
August	16	58.1	97	30	1.08	2.14	75.5	80	70	209	559	15
September	27	48.7	81	30	1.13	2.35	8.3	80	71	278	497	15
October	12	24.1	92	30	1.19	3.12	6.8	80	81	593	020	15
November	18	50.9	96	30	8.7	2.07	9.5	80	18	250	380	15
December	21	32.4	54	30	9.2	1.77	5.6	80	140	213	592	15

3. The Neural Network Simulator

In this section we give a detailed description of the proposed neural network simulator used to predict the impact of the chemical ingredients on air quality.

3.1. *The Artificial Neural networks description*

The Artificial Neural Network (ANN) is capable of learning the relationships between inputs (manipulated and disturbance variables) and outputs of the process based on its past history. The ANN usually involves very simple dynamical schemes as nodes, and very complex networks of connections, an approach known as connectionism. Once the neural model of the process is built, off-line trained, it can be continuously updated on-line, in real-time, by minimizing the difference between its predicted output value, Y, and its target value $\hat{Y}$. Their architectures, similar those presented in Figure 5-6 (Smith and Bonin (1997), Haykin (2001), Tudoroiu et al. (2006)), represent computational models that consist of a number of simple processing units (neurons), placed in layers (input, hidden, output) which communicate by sending signals to each other over a large number of weighted connections. The simplified network diagram shown in Figure 5 is a full-connected, four layers (input, output and two hidden) feed-forward, perceptron neural network. Full-connected means that the output from each input and hidden neuron is distributed to all of the neurons in the following layer and feed-forward means that the values only move from input to hidden to output layers; no values are fed back to earlier layers as a recurrent network does. The detailed full-connected, feed-forward, multilayer perceptron network diagram is shown in Figure 6.

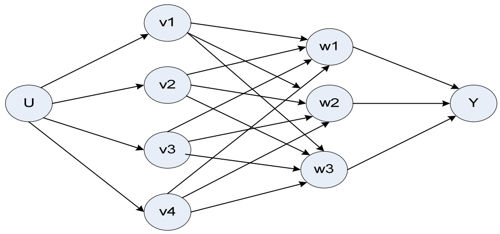

Fig.5.The simplified multilayer perceptron architecture having 1-4-3-1 neurons

All of these neural networks have an input layer and an output layer, but the number of hidden layers may vary as shown in Figures 5-6. When there is more than one hidden layer, the output from one hidden layer is fed into the next hidden layer and separate weights (matrix W) are applied to the sum going into each layer. The processing units transport incoming information on their outgoing connections to other units. The signal information is simulated with specific values stored in those weights w_{ij} that give these networks the capacity to learn, memorize, and create relationships among experimental input-output data sets. Each unit *j* can have one or more inputs, but only one output. An input to a unit is either the data from outside of the network, the output of another unit, or its own output. The total input to unit *j* is simply the weighted sum of the separate outputs from the connected units plus a threshold or bias term ($\theta_1, \theta_2, ..., \theta_n$).

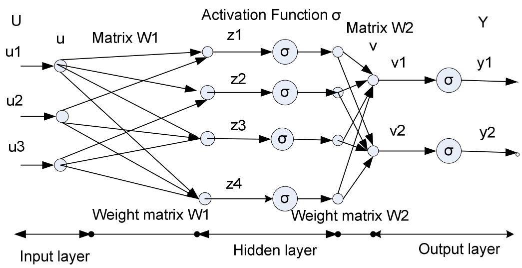

Fig.6.The detailed multilayer perceptron architecture having 3-4-2 neurons

Most of these units transform their net inputs by using a scalar-to-scalar function called an activation function σ (sigmoid function), given by:

$$\sigma = \frac{e^{ax}}{1+e^{ax}} \quad (1)$$

where a represents the learning rate of the neural network scheme. The "S" shape of the sigmoid curve corresponding to (1) is represented in Figure 7.

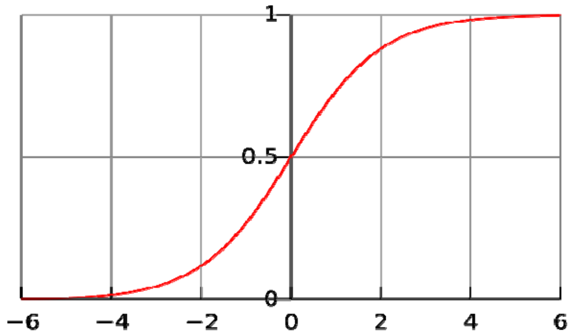

Fig. 7. The sigmoïde activation fonction

Recently, empirical models derived from neural networks have been shown to offer advantages in both accuracy and robustness over more traditional statistical approaches (regression methods).

3.2. *The Neural network back-propagation training scheme*

Our goal in this research is to determine appropriate neural-models for our air quality indicators. The experimental input-output data set will be used to train feed-forward neural networks using an error back-propagation algorithm. We will focus our attention on matching model predictions with measurements for network learning and generalization. For this purpose we will investigate the simulation with neural networks consisting of three layers (input, hidden, output) or more, configured in different architectures trained by the Levenberg-Marquardt back-propagation error algorithm (Bishop (1995); Haykin (2001); Tudoroiu et al. (2002),(2006); Zaherruddin (2004)). The number of hidden neurons and layers are varied to provide optimal network performance. The development of an optimal neural network structure is complicated by the fact that back-propagation networks contain several adjustable parameters for which the optimal values are initially unknown. These include structural parameters (such as the number of hidden layer neurons, initial weights and biases) as well as learning parameters (such as the learning rate, momentum, and error goal). The learning rate determines the speed of convergence by regulating the step size. However, the network may settle far away from the global minimum of the error surface if the learning rate is too large. On the other hand, smaller rates can ensure the stability of the network by diminishing the gradient of noise in the weights, but result in longer training times. For this reason the algorithm could be improved by introducing an adaptive learning scheme which decreases the training time considerably. A smaller training tolerance usually increases learning accuracy, but can also result in less generalization capability as well as longer training time. Conversely, a larger tolerance enhances convergence speed at the expense of accuracy in learning. It is shown in the literature that a single hidden layer is sufficient for learning any function, but the number of hidden neurons can grow without a bound.

This, of course, may result in a network with a large number of connections which defeats the main purpose of having an accurate prediction. By increasing the number of hidden layers, each consisting of sigmoid nodes, the complexity of the network can increase more rapidly than the number of connections. The optimum network architecture should have a minimum number of connections and produce a low cross-validation error. Development of neural network models typically consists of considerable training and testing. The objective is to find a network that will perform well on the test data. Network performance is measured by the root mean squared error (RMSE) (Khalid and Omatu (1990), May et al. (1991), Kim and May (1993)), which is given by:

$$\sigma = \sqrt{\frac{1}{n-1}\sum_{i=1}^{i=n}(y_i - \hat{y}_i)^2} \ . \tag{2}$$

where n is the size of the test set, y_i is the measured value of the output, and $\hat{y}_i$ is the estimated response provided by the neural networks. To avoid over fitting it is recommended to limit the number of neurons to the fewest possible, as long as the network converges to the desired error level, and cut off the training once that error is met. One of the problems that occurs the most in many applications could be the over-fitting. The error on the training set is driven to a very small value, but when new data are presented to the network, the error is large. The network has memorized the training examples, but it has not learned to generalize to new situations. One method for improving network generalization is to use a network that is just large enough to provide an adequate fit. If we use a small enough network, it will not have enough power to over-fit the data.

3.3. *The Neural network simulator results*

Several architectures of neural networks were developed in different successive layers with each layer having fewer units than the previous layer. Every time a new layer was built, a single unit, called the master unit, was added. Then step-by-step additional units were also added. At every step the neural network was trained and the forecasting performance was estimated. The whole process was repeated until a larger network did not sufficiently contribute to the forecasting performance. During the process of network design selection, we tested every neural network structure for different horizons; all calculations have been performed using MATLAB 7.5 (R2007b) software, Neural Network TOOLBOX. We used the back-propagation algorithm because automatically supervises the testing and records the neural network performance. After extensive testing of the possible structures of neural network designs, we selected the best neural network architecture that performed very well (trial and error procedure). The layers of a multilayer network play different roles. Multiple-layer networks are quite powerful. We underlined one important contribution of neural networks--namely their elegant ability to approximate arbitrary nonlinear functions. To avoid over fitting we limited the number of neurons to the fewest as possible as long as the network converges to the desired error level, and we cut off the training process once the error is met. In a simulation environment, in the absence of the perturbations, we found that our neural simulator performs well using a 6-30-1 structure, i.e. six input neurons, 30 hidden neurons, and an output neuron. In the presence of the perturbations, according to the number of input perturbations considered, we found that 7-30-1 (one perturbation input), 8-30-1 (two perturbation inputs), 9-30-1 (three perturbation inputs) structures are more suitable to be used. The neural network inputs of all these structures are represented by the air pollution agents (the input concentrations of NO_2, NH_3, CO, O_3, C_6H_6, PM_{10} from Tables 1 and 2) and the perturbations such as the temperature, rainfall and the wind speed. The neural network output is represented by the air mixture concentration. Before training the network weights and biases are initialized off-line using Nguyen-Widrow initial conditions (small random values). Also the network parameters are initialized by the following values: error goal = 0.025, learning rate = 0.02 and momentum = 0.95. For each structure the back-propagation algorithm attempts to minimize the error between the output of the network and the target or desired response in weight space, using the method of gradient descent in conjunction with Levenberg-Marquardt relaxation (Haykin (2001), Tudoroiu and Patel (2006)). In this research we studied the following possible situations:

3.1.1. *The air mixture concentration in the absence of the disturbances*

The simulation results are presented in Figures 8-13.

In Figures 8-9, the validation model and the learning curve in the absence of the disturbances are represented. In Figures 10-12, the neural models of the air mixture concentration (minimum, maximum, average, maximum permissible values) in the absence of the disturbances are represented. From these simulation results, we noticed the experimental data set had a very good capacity of learning input-output map, and a very good capacity of generalization. For comparison purpose we represent in figure 13 all these neural models in the same graph. Also in this graph we could see the permissible value of the air mixture concentration, given by the European standards.

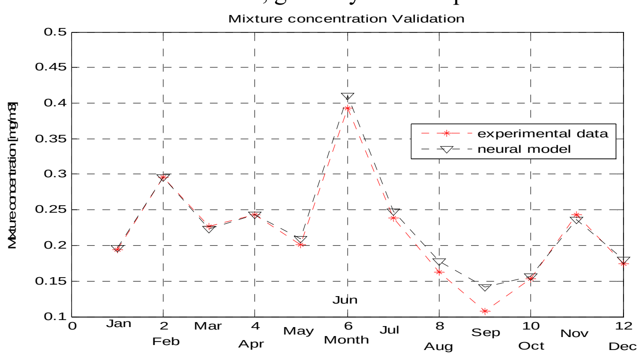

Fig.8.The mixture concentration validation without disturbances

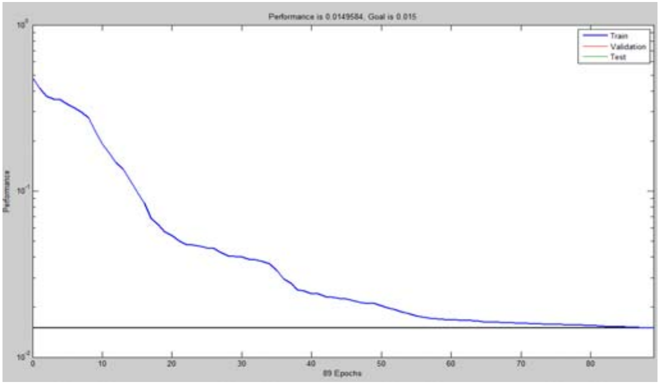

Fig.9.The learning curve in the absence of the disturbances

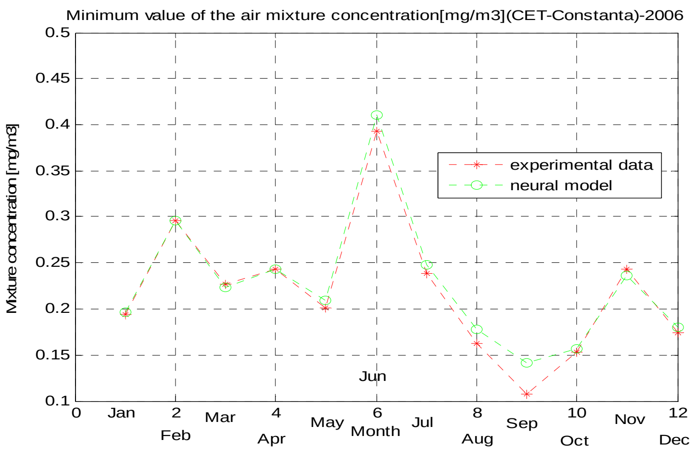

Fig.10.The minimum value of the air mixture concentration in the absence of the disturbances

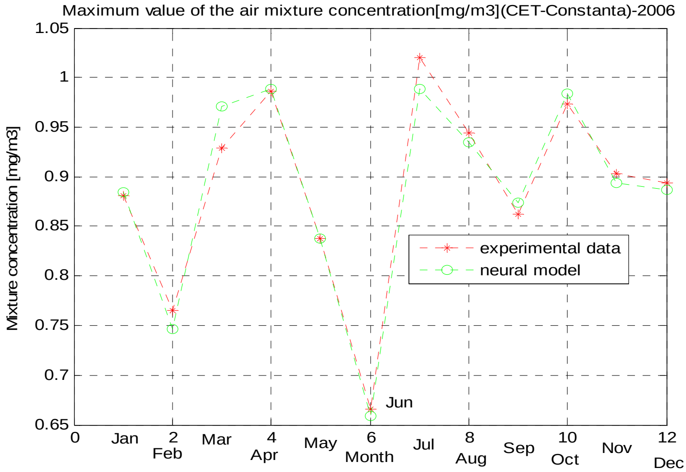

Fig.11.The maximum value of the air mixture concentration in the absence of the disturbances

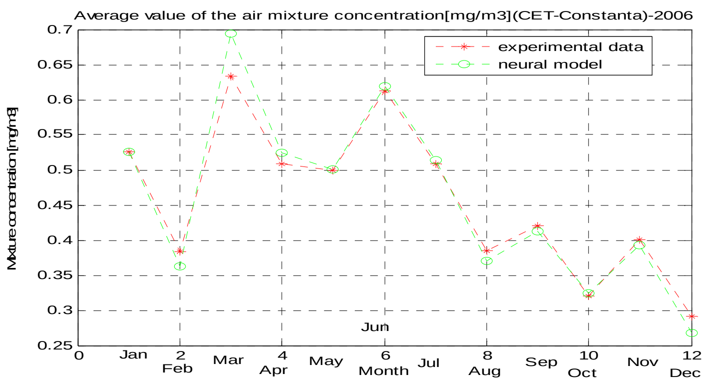

Fig.12.The average value of the air mixture concentration in the absence of the disturbances

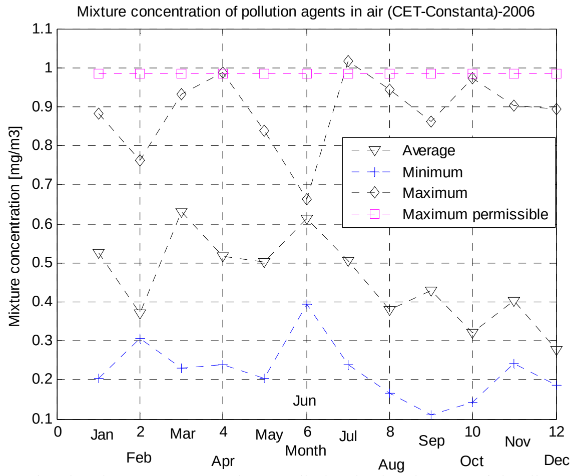

Fig.13.The air mixture concentration prediction in the absence of the disturbances

3.1.2. *The air mixture concentration with the temperature changes effect*

In this situation we will take into consideration the effect of the temperature changes on the global characteristics of the air mixture concentration. The simulation results are presented in Figures 14-16.

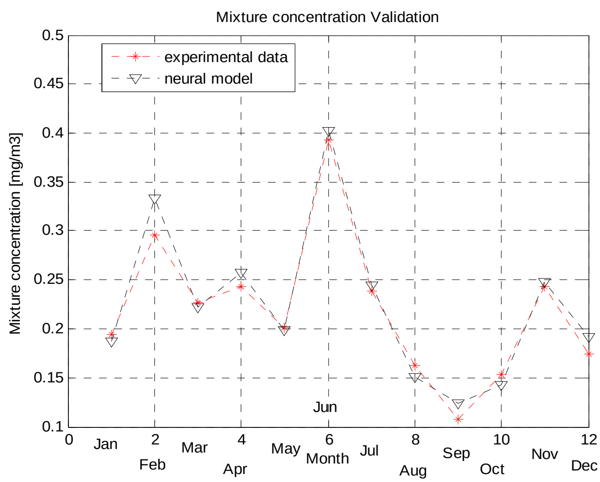

Fig.14.The mixture concentration validation in the presence of the temperature changes

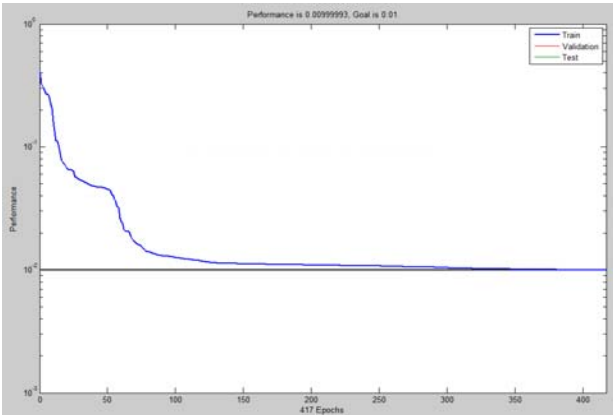

Fig.15.The learning curve in the presence of the temperature changes

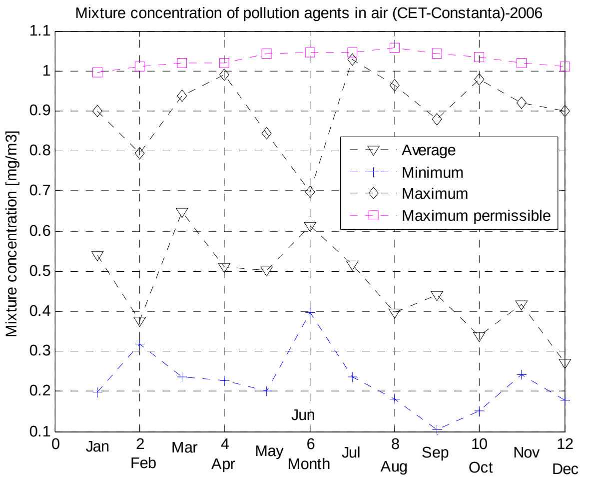

Fig.16.The air mixture concentration prediction in the presence of the temperature changes

Compared to the air mixture concentration in the absence of the disturbances represented in Figure 13, the effect of the temperature changes represented in Figure 16 becomes significant during the period April, June, August, September and December.

3.1.3. *The air mixture concentration in the presence of rainfall*

For this case we will take into consideration the effect of rainfall on the air mixture concentration characteristics. The simulation results presented in Figures 17-19 (validation, learning curve and prediction) reveal significant changes for the period July, October and December.

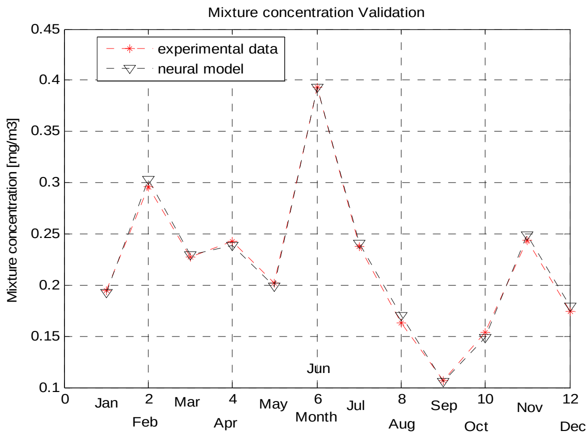

Fig.17.The mixture concentration validation in the presence of rainfall

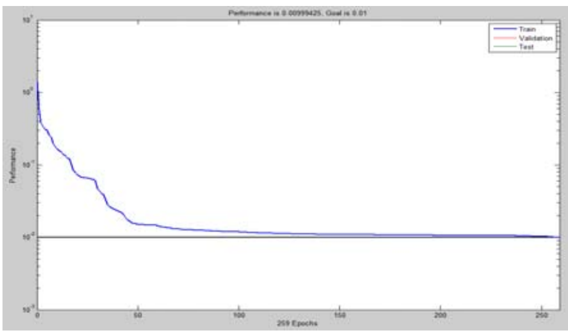

Fig.18.The learning curve in the presence of rainfall

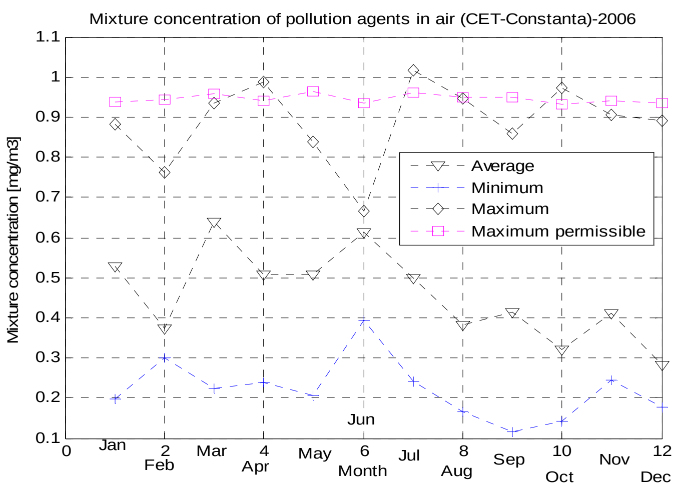

Fig.19.The air mixture concentration prediction in the presence of rainfall

3.1.4. *The air mixture concentration in the presence of the wind*

In this situation we will take into consideration the effect of the wind speed on the air mixture concentration characteristics. The simulation results are presented in Figures 20-22 (validation, learning curve, prediction) and reveal significant changes, especially in maximum permissible value for the period April, June, October and December.

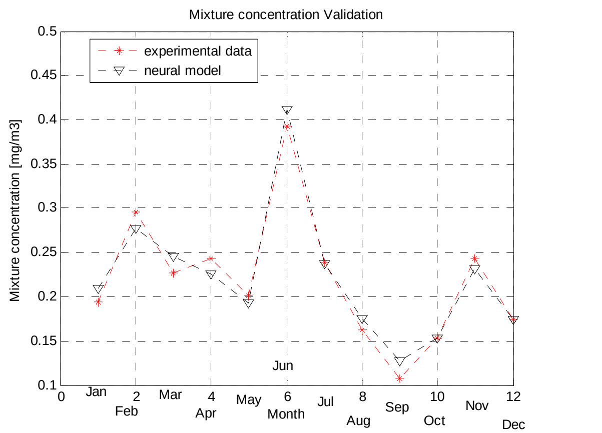

Fig.20.The air mixture concentration validation in the presence of the wind speed

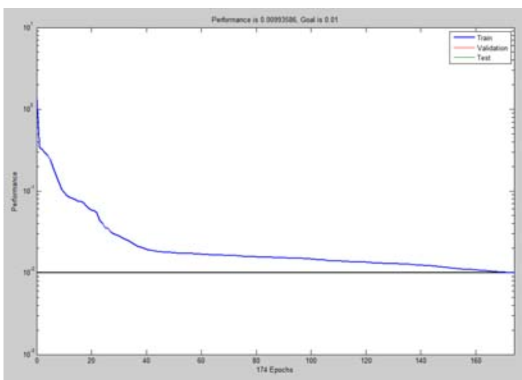

Fig.21.The learning curve in the presence of the wind speed

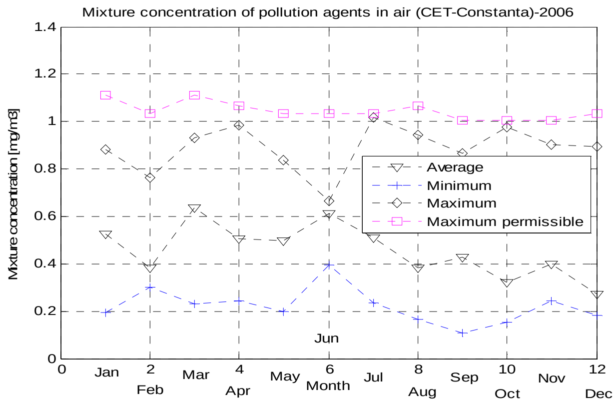

Fig.22.The air mixture concentration prediction in the presence of wind speed

In Figures 23-25 we present a special scenario when the wind had high speed intensity (storm) during some days of 2006 (validation, learning curve, prediction). We notice significant changes for the days where the wind had high speed intensity from February, April, June, July, September and December.

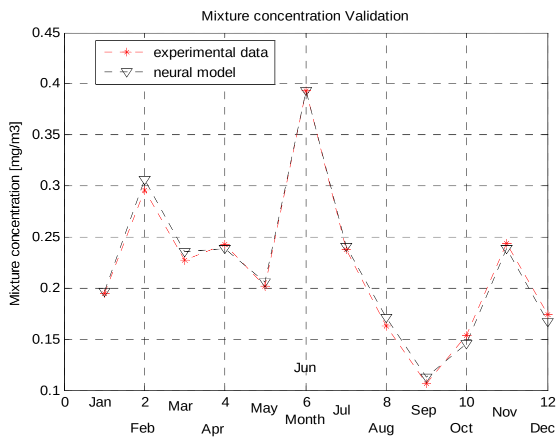

Fig.23.The air mixture concentration validation in the presence of the storm

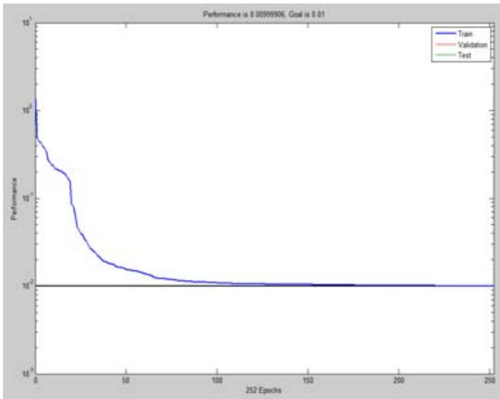

Fig.24.The learning curve in the presence of the storm

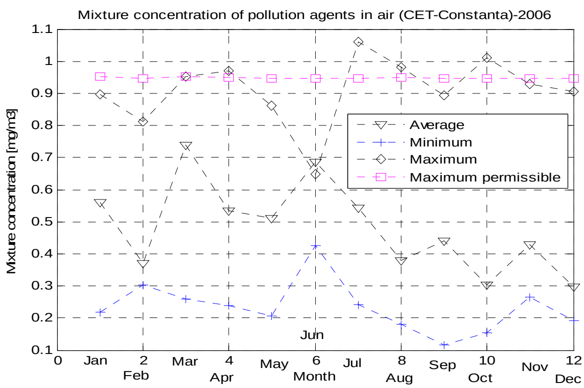

Fig.25.The air mixture concentration prediction in the presence of the storm

3.1.5. *The air mixture concentration in the presence of all of the disturbances (temperature, rainfall and wind speed)*

In this scenario we take into consideration the effect of all these perturbations (temperature, rainfall and wind speed) on the air mixture concentration characteristics. The simulation results are presented in the Figures 26-28 (validation, learning curve, prediction) and reveal significant changes, especially for the period March, July, September, November and December.

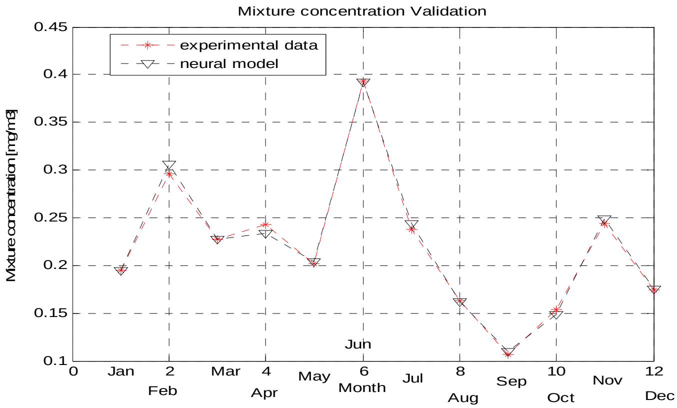

Fig.26.The air mixture concentration validation in the presence of all disturbances

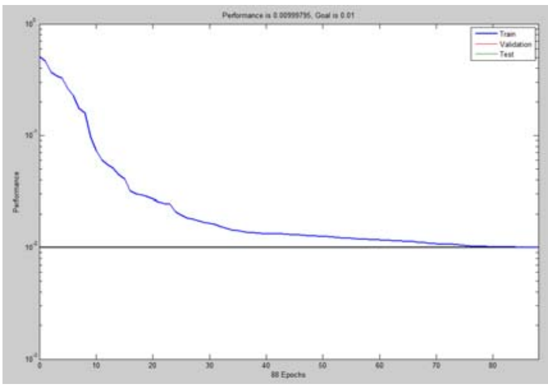

Fig.27.The air mixture concentration validation in the presence of all disturbances

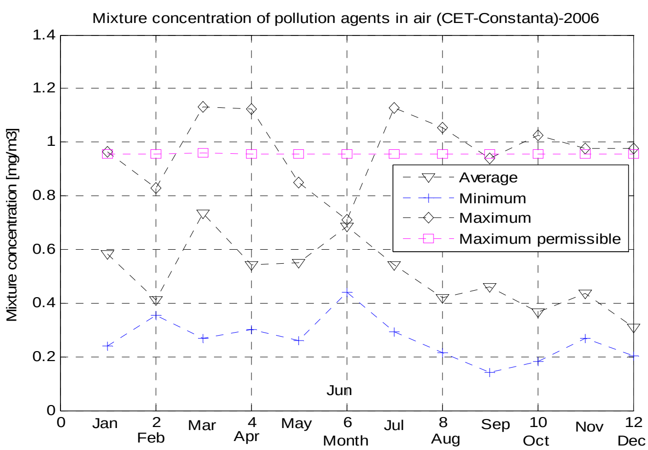

Fig.28.The air mixture concentration prediction in the presence of all disturbances

4. Conclusion

This research work is dedicated to investigate the possibility of applying several neural network architectures for the simulation and prediction of the performance of air quality of the Constanta Black Sea resort city environment. Therefore we explore different neural network architectures to build several neural models based on the experimental data set provided by the "in-situ" samples measurements sites. Due to the black box nature of neural networks, users of forecasts may feel some discomfort if they are unable to give proper physical interpretation to the estimated relationships. Also it is very difficult to determine which of the explanatory variables are driving the bulk of the forecasts, as comparative statistics are difficult to perform. On the other hand it is very difficult to yield a specific functional form that is to be used for empirical verification of the theory. In such cases, neural networks have a great advantage over traditional methods. A researcher can start with a large network and prune it to the most efficient form.

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