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USING OF ARTIFICIAL NEURAL NETWORKS IN PREDICTIONS OF SO_2, NO AND NO_2 CONCENTRATIONS IN GLIWICE, POLAND

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PREDYKCJA STĘŻEŃ SO_2, NO I NO_2 W GLIWICACH Z UŻYCIEM SZTUCZNYCH SIECI NEURONOWYCH

W niniejszej pracy posłużono się wynikami pomiarów warunków meteorologicznych do wygenerowania sieci neuronowych prognozujących wartość stężenia na podstawie znajomości warunków meteorologicznych. Wyniki pomiarów obejmują: stężenia trzydziestominutowe: SO_2, NO, NO_2, parametry meteorologiczne: kierunek i prędkość wiatru, temperatura powietrza, natężenie promieniowania słonecznego, wilgotność powietrza i klasa stabilności atmosfery. Do analizy danych zastosowano program Statistica Neural Networks firmy StatSoft. Proces uczenia przeprowadzono stosując algorytm Levenberga – Marquardta. Dla celów prognozy zanieczyszczeń (SO_2, NO_2, NO) stworzono, wyuczono i przetestowano około 600 sieci dla każdej substancji i z nich wybrano trzy najlepsze. Wybrane sieci zostały wykorzystane do przewidywania wartości stężeń na podstawie parametrów meteorologicznych. Kolejno uruchamiano modele neuronowe dla: SO_2, NO, NO_2. Sporządzono, dla każdego zanieczyszczenia, wykresy przedstawiające przebiegi stężenia rzeczywistego i prognozowanego oraz wykresy błędu, jaki popełnia sieć podczas predykcji kolejnych stężeń.

Summary

The paper presents application of measurements of pollutant concentrations and meteorological conditions to create neural networks able to predict the pollutant concentrations on the basis of meteorological conditions. The measured quantities comprised 30-min concentrations of SO_2, NO, NO_2 and meteorological parameters, such as direction and speed of wind, air temperature, solar radiation, air humidity, and Pasquill stability class of atmosphere. The data were developed with the use of the StatSoft's Statistica Neural Networks computer program. The Levenberg – Marquardt algorithm was used to train networks. About 600 networks were created, trained and tested for each of SO_2, NO and NO_2 to predict their concentrations in ambient air and from among them the best performing network was selected. The chosen networks were used to compute concentrations on the basis of meteorological parameters. The neural models were run subsequently for SO_2, NO and NO_2. Measured and computed concentrations of the pollutants were presented in charts, as well as errors made by networks while predicting.

INTRODUCTION

The Silesian Agglomeration, a great association of 16 cities, lies in the central part of Silesia. The city of Gliwice, a greater one in the Agglomeration, occupies about 134 km^2

(over 10% of the Agglomeration area) in its western part. The population density of Gliwice is 1504.5 people per square kilometer (average for Poland in 2003 was 122 persons per square kilometer) [18]. Gliwice has very compact building arrangement, especially in downtown. Main traffic streams run through the central part of the city – there are no circular routes bypassing the city round. Street ventilation of the city central part is poor, which is of special importance in rush hours, when the city is practically paralyzed by one, big and permanent traffic jam, and vehicular pollution reaches its extremes [12, 23, 24].

The main ambient air pollution sources in Gliwice are industry, municipal sources, "low emission" from domestic furnaces and motor vehicles. Also, but rather in small amounts, contaminants migrate from neighboring areas [12].

The highest concentrations of pollutants in Gliwice occur in heating season (1995–2000) [12], and as it especially concerns SO_2, suspended dust, NO_x and CO, the pollution is attributed to heating systems using solid fuels, i.e. the electro-power station and domestic furnaces. However, in Gliwice the greatest all-year-round emission source is the traffic, contributing about 25% of NO_x and CO, and 60% of aromatic hydrocarbons to total emission to the atmosphere [12, 23, 24]. Such a situation is caused by insufficiently developed communication system allowing heavy truck transport to run through the city.

In Gliwice, within frames of the Regional Air Quality Monitoring program, concentrations of the main air pollutants are measured by the automatic station installed in Kujawska Street. It yields vast sets of data every year. The data had been used merely for the air quality evaluation, but about 10 years ago the idea of using it in predictions of the air pollution emerged. The basic tool for predicting concentrations of air pollutants was the Artificial Neural Networks (ANNs).

Applications of the ANNs in air protection, and especially in air pollution forecasting, are reviewed by Gardner and Dorling [6]. Among many types of ANNs, the most often applied and important one is a one way (i.e. feed-forward), multilayer network with sigmoid neurons, referred to as the Multilayer Perceptron (MLP) in the literature. In those networks information flows in one direction – from input to output. Training methods for MLPs are simple and easy to implement – usually an MLP is trained with a supervisor (error backpropagation method and its modifications [22, 27], RLS algorithms [4], Levenberg – Marquardt algorithm [22, 27]).

In 1993, Bonzar [3] presented possibility of the MLP application in predicting SO_2 concentrations in ambient air on the basis of meteorological data. The data came from a heavily urbanized area of Slovenia. In 1999, Gardner and Dorling [7] published a paper on prediction of 24 h concentrations of NO_x and NO_2 in London, where they used perceptrons, and discussed the advantages of their method over regression models. Perez in his papers proved and broadly discussed applicability of the neural models in prediction of the air pollution. In 2000, he used a three layer perceptron to predict $PM_{2.5}$ concentrations in atmospheric air in Santiago, Chile. Beside the standard meteorological parameters, as an additional input variable he used the $PM_{2.5}$ concentration measured the day before [11]. Perez made prognoses of NO_2 concentrations in air in vicinity of very busy streets using two additional inputs: the air temperature predicted for the time of anticipated NO occurrence and NO concentrations measured several hours before this time [10]. In [9], Perez presented application of the three layer perceptron in forecasting the SO_2 concentrations in the air. He obtained the best results by using – beside the standard inputs, i.e. meteorological data – SO_2 concentrations measured 6 hours before the time the concentration prognosis was to

be done for. Andretta et al. [1], using SO_2 concentrations and meteorological data as the network inputs, predicted exceeding of admissible air concentrations of SO_2. The network output was binary: it issued 1 if the concentration exceeded 40 $\mu g/m^3$, otherwise 0.

The present paper describes an attempt to predict air pollution in Gliwice at the site monitored by the automatic station (station A5 of the Regional Air Pollution System Monitoring). The station is located within the premises of the Silesian Technical University in Gliwice. Its geographic coordinates are: longitude 18°41'03"E, latitude 50°17'07"N, altitude 232 m over the see level. The nearest pollution sources were:

- Chemical Works CARBOCHEM – about 1300 m SE,
- Hard Coal Mine GLIWICE – about 500 m S,
- Steel Works "1-go MAJA" – about 1300 m N,
- Electro-Power Station GLIWICE – about 2000 m NE,
- Hard Coal Mine SOŚNICA – about 2200 m E,
- Domestic furnaces of downtown – in a circular sector from west to north.

The station was equipped with:

- CO analyzer ML 8830,
- NO_x analyzer ML 8841,
- SO_2 analyzer ML 8850S,
- Suspended dust analyzer TEOM 1400,
- Speed and direction of wind sensor KRONEIS,
- Air temperature sensor KRONEIS,
- Air humidity sensor KRONEIS,
- Solar radiation sensor KRONEIS.

Air pollutants typical of heavily urbanized and industrialized areas were investigated:

- Sulphur dioxide, SO_2, – in ambient air comes from combustion of fuels contaminated with sulphur: solid (hard coal) in power and electro-power stations, liquid (oils) in car engines,
- Nitrogen dioxide, NO_2, and nitrogen oxide, NO, – excessive amounts of those gases in the atmosphere come from the production processes (high temperature technologies, power station furnaces) and car engines.

Anthropogenic sources may emit up to 90% of SO_2 and NO_x into the atmosphere in such areas [19], although this figure may not be adequate to many regions due to insufficiently recognized emissions (especially low emission from domestic sources and traffic) and transport of air contaminants.

The scope of works done within the undertaken task was following:

- Transforming raw numerical data into arrays possible to be introduced into the program,
- Detailed pre-processing of data [16, 21],
- Testing subsequently built networks for their predictive abilities (training, validating, and testing various networks by presenting them with selected data sets),
- Choosing the best, respect to proper criteria, neural network,
- Applying an ANN to prediction of air pollutant concentrations on the basis of given meteorological parameters,
- Analyzing the results; comparing computed (predicted) concentrations with measurements.

The StatSoft's Statistica Neural Networks computer program, simulating the ANN

performance, was used to complete all the tasks. The Levenberg – Marquardt algorithm was used to train the networks [22, 27].

THE DATA FILE

Measured data consisted of 30-min concentrations of sulphur dioxide (SO_2), nitrogen oxide (NO), nitrogen dioxide (NO_2) in ambient air, as well as meteorological parameters such as speed and direction of wind, air temperature, solar radiation and relative air humidity. Additional information, computed from data provided by the Institute of Meteorology and Water Resources (IMWR), was Pasquill stability class of atmosphere [8, 14]. The data covered the period from January 5 to December 31, 1996.

The data statistical parameters were following:

Measured parameter		Range of changes	Mean	Standard deviation
Wind direction	°	61–89	77	8.3
Wind speed	m/s	0–6.3	2.4	1.45
Air temperature	°C	23–30.3	2.9	10.4
Relative humidity	%	25–96	74	17.2
Solar radiation	W/m^2	0–924	104.2	188.2
Atmosphere stability category	-	1–6	–	–
SO_2 concentration	$\mu g/m^3$	6–303	74.7	45.5
NO_2 concentration	$\mu g/m^3$	11–147	44.7	17.0
NO concentration	$\mu g/m^3$	1–382	18.3	28.4

Values of the above meteorological parameters, together with proper concentration of one of the three pollutants, constituted the basic record of data to that pollutant. In the experiment, 1460 such records, i.e. 1460 various meteorological situations, were used for each of NO, NO_2, and SO_2.

CREATING NEURAL MODELS

For each of the three pollutants, NO, NO_2, and SO_2, the array built of 1460 basic records was prepared. Each basic record contained 30–min measurements of meteorological parameters and proper 30–min concentration of a particular pollutant.

The ST Neural Network data file editor was applied to the data.

The input and output variables were chosen. The input variables were the meteorological parameters, the output variable, in every case, was the concentration of a pollutant. Designed networks had six input variables (air temperature, relative air humidity, wind direction, wind speed, Pasquill atmosphere stability category, and solar radiation) and one output variable (concentration of SO_2, NO_2 or NO).

Network training demands dividing of the data set into three parts: training, validating and testing subsets. The editor window has three fields, each comprising a number of records of one of these sets. The testing subset is created to arbitrarily evaluate the network performance after the designing and training phases. In the presented case, the subsets were built of records randomly chosen from the main data set (possibility of mixing of records was provided by the used software).

The next step in the network designing was transforming the raw data into numerical data, acceptable to the network for further development, and the network output value into

a value corresponding with the raw data format (pre- and post-processing) [15, 17, 25].

Once the data arrays were loaded into the program, the ANNs resulted from the standard sequence of the following operations:

- Choosing an initial structure of a network (a network with one hidden layer and an initial number of hidden neurons being half the sum of numbers of input and output neurons);
- Choosing the best network configuration (in respect of a validating error determined for a validating sequence) by iteratively experimenting with each of all possible configurations;
- Attempting addition of new neurons to the hidden layer (or whole hidden layer) if the experiments proved under-learning of the network (the network did not reach assumed error level);
- Attempting removal of some number of hidden neurons (or whole hidden layer) if the over-learning (the model fits the data from the training set too well; the ANN loses its generalization abilities) of the network occurred (validating error had considerably increased before the network was sufficiently trained); the training records were also added.

In the last step, a linear network was sought to forecast the value of the particular output variable (concentration), having the error comparable to error of the best MLP. There exist many problems that are not solvable by using linear methods. However, in many applications the linear methods perform very well. Due to their simplicity and easiness of use they should be chosen even in case they give slightly worse effects [17, 22, 27].

In the whole process of looking for the best performing network, 600 models, differing from each other with their architecture, for each of the three pollutants and all data sets were tested [13]. The criteria to select the best neural networks were following:

General estimate: Automatically reported by ST Neural Networks as exceptionally bad, very bad, bad, OK, good, very good, excellent [16, 17].

Regression coefficient: (proportion of standard deviations). It is called sometimes the quality of a network. If it is greater than or equal to 1, then the model yields results not better than the model outputting always the same signal being simply the mean of the earlier observed input values. Value less than 1 means the model having better output fitting – the lower regression coefficient, the better the model.

Correlation: The coefficient expressing relation between values of concentrations on input and output of a network; it varies within the interval 0–1; the closer the correlation to 1, the higher quality of the received network [2, 22].

Network error: The network error is the square root of the sum of squares of the errors determined by the network error function for basic records. If in the process of creation of networks the training, validating and testing sets are formed, then, while learning, the errors are determined for each of those sets, but only the error computed for the validating set is referred to while training. Increasing of this error at some step of the training means the network over-learning. The error computed for the testing set is the ultimate criterion to verify the network. The selected network is the best one in respect of the validating set error [2, 17, 22, 27].

When the network error and network general estimate were close, the network was selected with respect to the correlation.

NEURAL MODELS

Below, in Table 1, the neural networks selected to predict concentrations of pollutants and, in Figure 1, the general scheme of the network are presented.

Table 1. The best neural networks and their basic parameters

Output variable	Type	Structure	General estimate	Regression coefficient	Correlation	Error
SO_2	LNN	6:40 -1:1	good	0.69	0.72	22.82
NO	MLP	6:40 -6-1:1	OK.	0.80	0.60	13.86
NO_2	MLP	6:40 -12-4-1:1	OK.	0.91	0.75	8.82

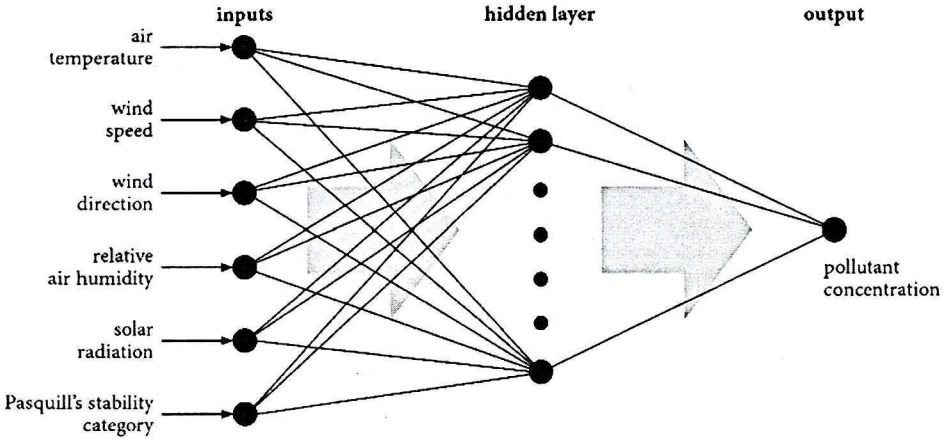

Fig. 1. Architecture of the three-layer feed-forward network applied in the study

Three-layer network was created for NO – it is presented in Figure 2 in detail. The network created for NO_2 is presented in Figure 3, for SO_2 – in Figure 4; all the three networks have the same number of inputs.

NEURAL NETWORKS IN PREDICTION OF POLLUTANT CONCENTRATIONS

After selecting and training the network once, its performance in predictions of concentrations of air pollutants was tested.

The trained network, applying acquired knowledge to the whole data set, computes concentrations of pollutants for given meteorological parameters. Results of computations are given in arrays; the fragment of one of them is presented in Table 2.

The results were used to draw charts of real and computed concentrations of particular pollutants. Comparative analysis of real and computed concentrations allowed evaluating performance of the network for each of the considered pollutants.

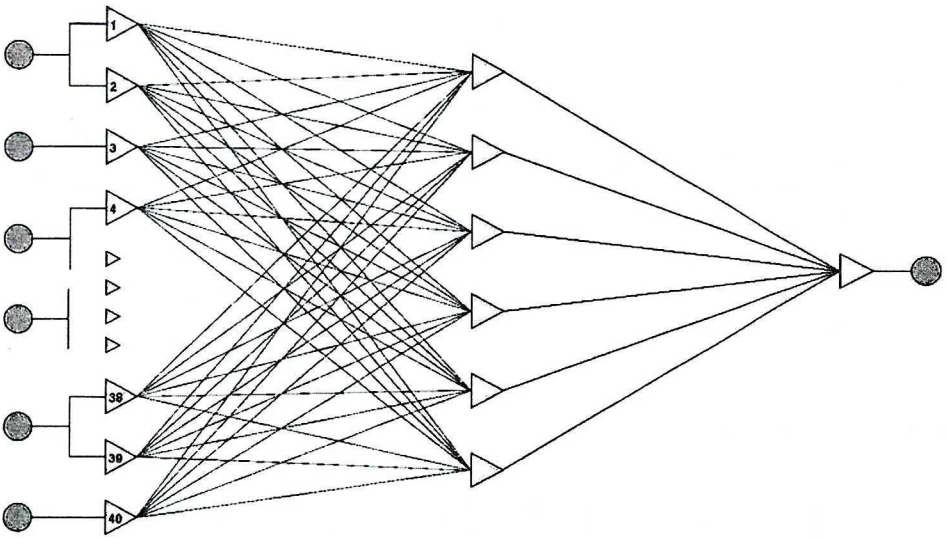

Fig. 2. Scheme of the network for predicting NO concentrations

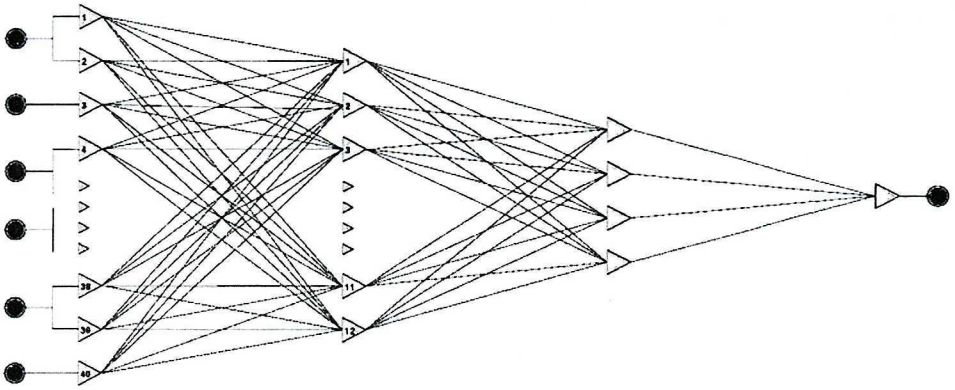

Fig. 3. Scheme of the network for predicting NO_2 concentrations

Running the network for NO yielded the array of resulting concentrations. On its basis, Figure 5 was made to compare real (measured) and predicted concentrations. For every base data record, the values of real and computed NO concentrations are different but trends of the two concentration functions are similar. Generally, the computations overestimated concentrations. The negative values of computed concentrations were very surprising because all the measured concentrations the network was trained and verified with were positive. Although the mean values of real and computed concentrations are close (18.44 $\mu g/m^3$ and 18.30 $\mu g/m^3$, respectively), their highest and lowest values differ considerably. The lowest computed concentration is – 19.65 $\mu g/m^3$, the lowest real one is 1 $\mu g/m^3$. The highest computed concentration is 142.06 $\mu g/m^3$, the highest real one is 382.0 $\mu g/m^3$. The maximum difference between real and computed concentrations is almost

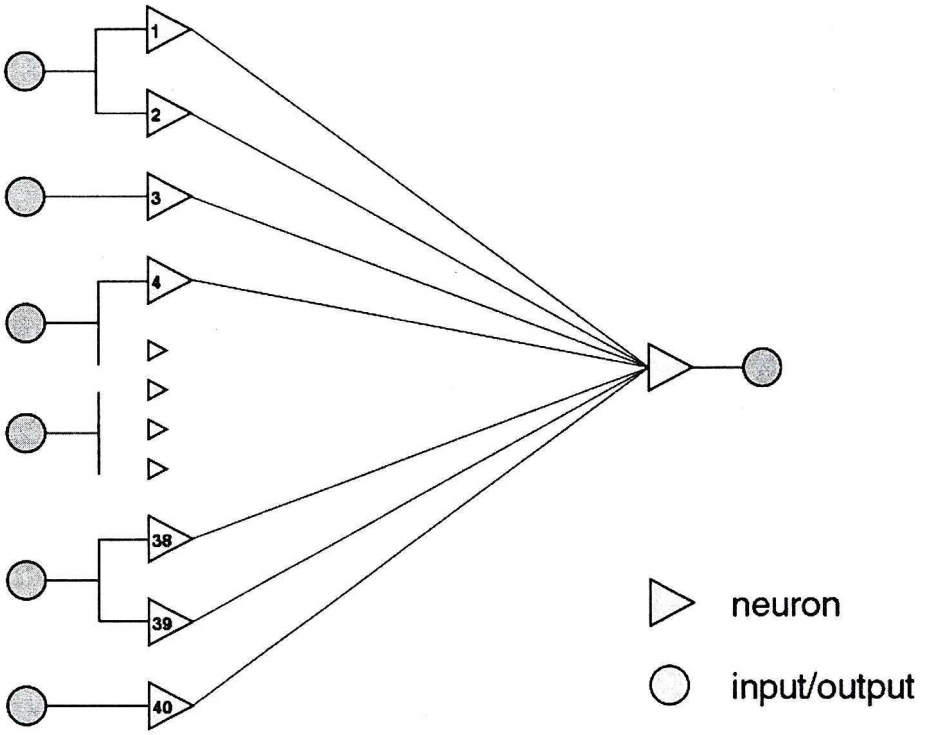

Fig. 4. Scheme of the network for predicting SO_2 concentrations

200.0 μg/m³. However, for many records concentration is computed with great accuracy – achieving even 0.002 μg/m³. The mean difference between real and computed concentrations is 13.35 μg/m³ – it is comparable with the mean concentrations. The most erroneous concentrations are computed for records with very high or very low real concentrations. It is due to using the Sum of Squares function as the error function. This function is very sensitive to particular cases and favors untypical records [22, 27]. The City Block error function [17], summing absolute values of differences between measured and computed concentrations instead of their squares was tried as a function computing the network error. Getting rid of the square dependence in the error function lowered the network sensitivity to untypical cases and the greatest values of errors dropped [15]. However, in other cases the errors increased. So, the error function was decided to be left unchanged. Supposedly, the best solution would be removing untypical records from the data set and training and running the network again. Because such data items were too numerous, such an action was given up in view of considerable reduction of the data set.

A plot of the RMS error was done (Fig. 6). From the plot it may be concluded that despite of the mentioned deficiencies, the network has quite good predictive properties for the whole data set. For the whole data set the RMS error is low. The error never reaches 0.8, and in most cases it is several times lower, which means good network performance in the given regression problem.

Table 2. The way of presenting results of computations (concentrations of NO)

No.	Real concentration [μg/m³]	Computed concentration [μg/m³]	Difference between computed and real concentrations [μg/m³]	Prediction error
1.	9	13.30	4.30	0.0113
2.	8	23.51	15.51	0.0407
3.	56	68.77	12.77	0.0335
4.	64	37.77	-26.29	0.0690
5.	10	27.12	17.12	0.0449
6.	50	70.39	20.39	0.0535
7.	13	8.84	-4.16	0.0109

In Figure 7, a comparison of real and computed by the network SO_2 concentrations is presented. Real and computed concentrations of SO_2 are close. Differences between the concentrations are small. Averaging real and computed concentrations gave almost equal figures (76.29 μg/m³ and 76.19 μg/m³, respectively). The highest concentrations differ – the real highest concentration is 303.0 μg/m³, the computed one is 263.49 μg/m³. The lower limits are also close except for negative values appearing among computed concentrations.

Averaged difference between real and computed concentrations is small (0.16 μg/m³), maximum difference between the two concentrations is 94.53 μg/m³, what makes about 33% of the maximum real concentration.

In general, the RMS error the chart of which is presented in Figure 8 oscillates between 0 and 0.25. Incidentally, the error reaches 0.7. The RMS error assumes such high values for records with very high real concentrations (computed, i.e. predicted, values are much lower).

Concluding, in spite of selecting a simple linear network, results of the prognosis of SO_2 concentrations are very good. The network performance was very good in predicting SO_2 concentrations.

The real and computed concentrations of NO_2 are compared in Figure 9. There exist some slight differences between the two concentrations. Averaged concentrations, real and computed, are almost equal (real: – 45.13 μg/m³, computed: – 45.07 μg/m³). Also the highest concentrations are similar: the highest real concentration is 147 μg/m³, the computed one is 147.17 μg/m³. However, the lowest real NO_2 concentration was 11 μg/m³ and the lowest computed one was equal to 17 μg/m³. The negative values of the computed concentration did not appear this time. Averaged difference between the real and computed concentrations of NO_2 is small and equal to 8.95 μg/m³. Minimum difference between the two concentrations is 0.003 μg/m³, and maximum difference between them is 48.79 μg/m³. The RMS error (Fig. 10) varies between $5.6 \cdot 10^{-7}$ and 0.36. Greater values of error, reaching the maximum, appear rarely and only for records with very high real concentrations (network foresees considerably lower concentrations).

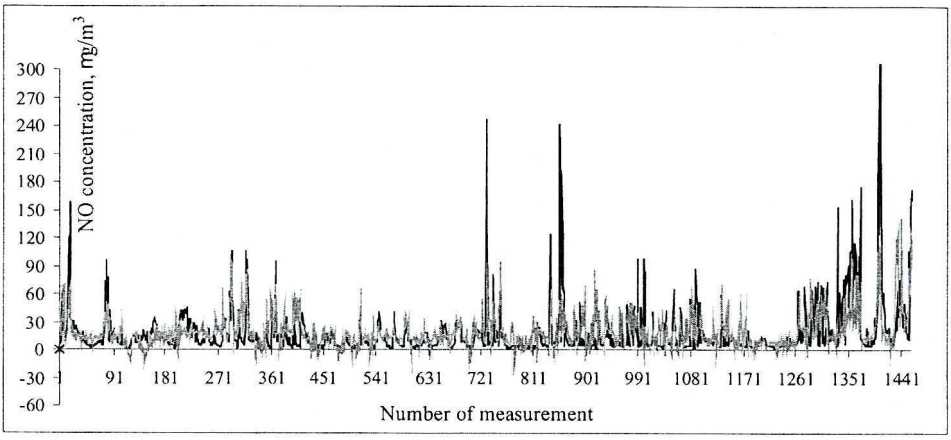

Fig. 5. Real and computed NO concentrations

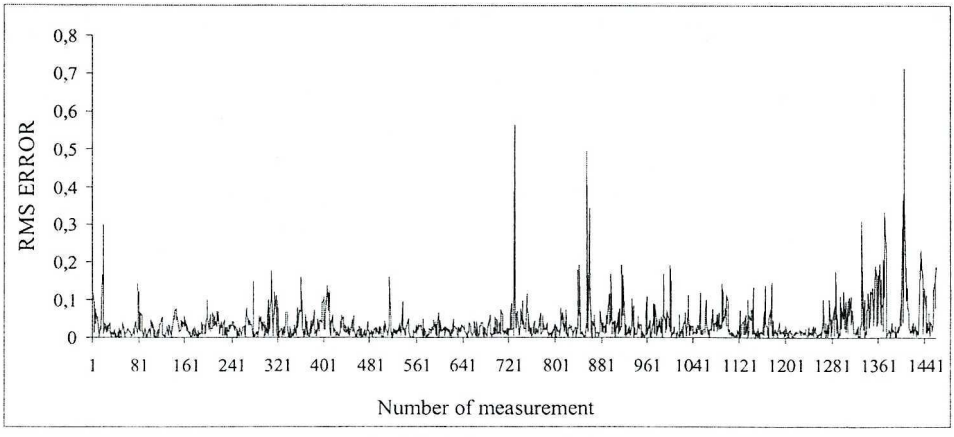

Fig. 6. RMS error for NO

CONCLUSION

The paper confirms possibility of predictions of air pollutant concentrations by applying the ANN to forecasted meteorological parameters. The neural models built for NO, SO_2 and NO_2 show quite good predictive abilities.

Both mean concentrations, computed and real, are close – often differing by no more than 2%. Trends of time variability of computed and real concentrations are the same for all the pollutants. Despite of this, the highest and lowest concentrations significantly differ. The chart of the computed concentrations against time is flattened and extremes are mitigated.

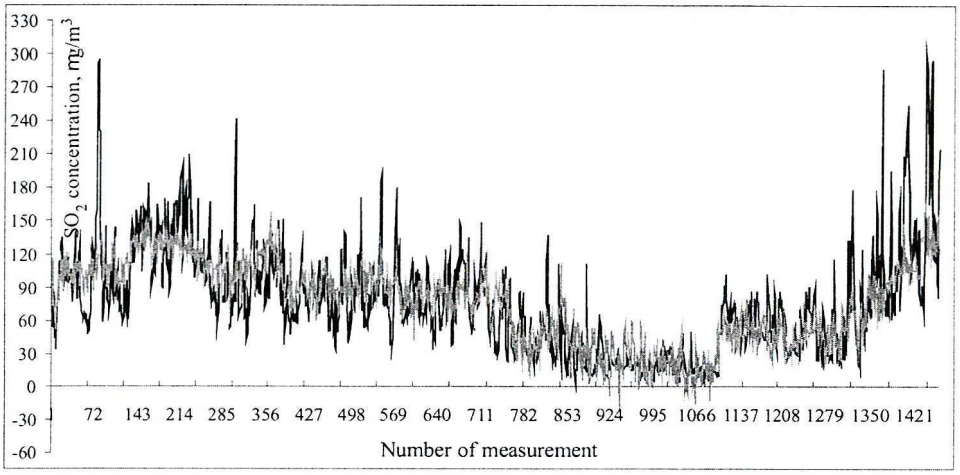

Fig. 7. Real and computed SO_2 concentrations

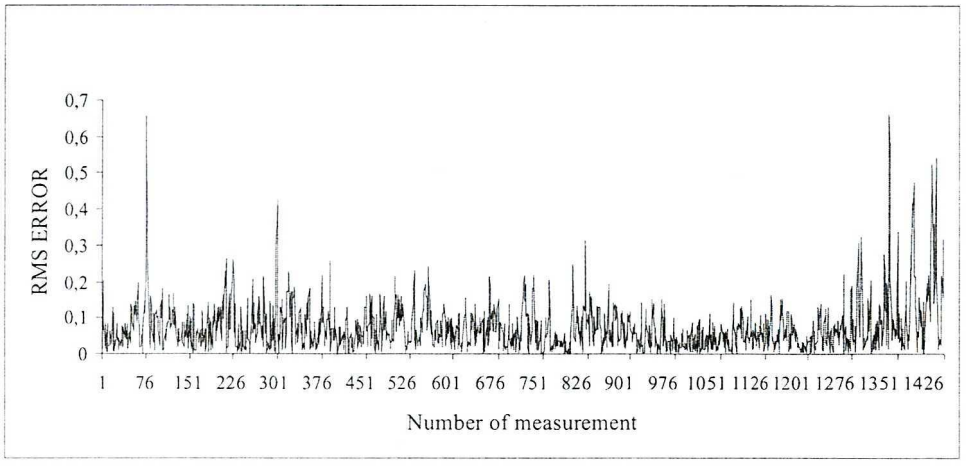

Fig. 8. RMS error for SO_2

Appearance of negative values in the set of computed concentrations may be considered a surprising curiosity. They occurred in spite of training and testing the network on the sets of measured data – i.e. the positive values. The appearance of the negative values was due to the situation where the network attempted to compute concentrations much higher or much lower than the mean. This is why difficulties in computing extreme values of concentrations should be considered a deficiency of the received neural models. It is rather unquestionable that these models can neither be used to predict instantaneous concentrations nor their maximum values. To build better neural models one should use

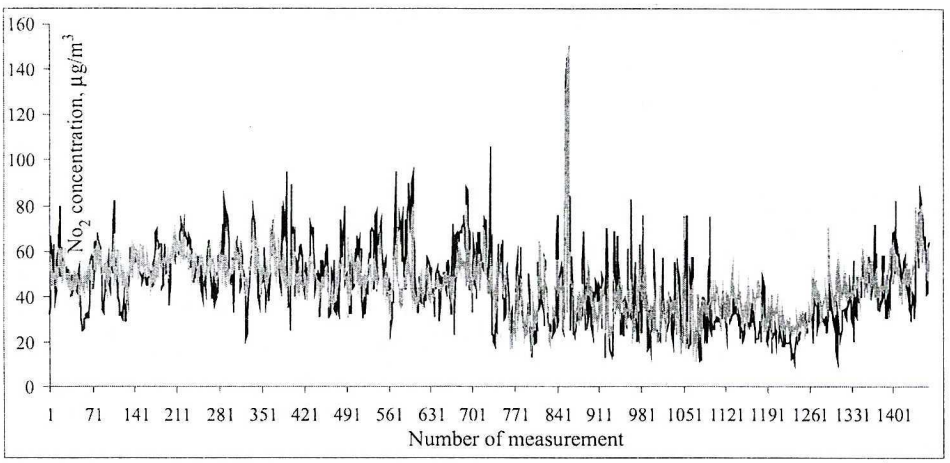

Fig. 9. Real and computed NO_2 concentrations

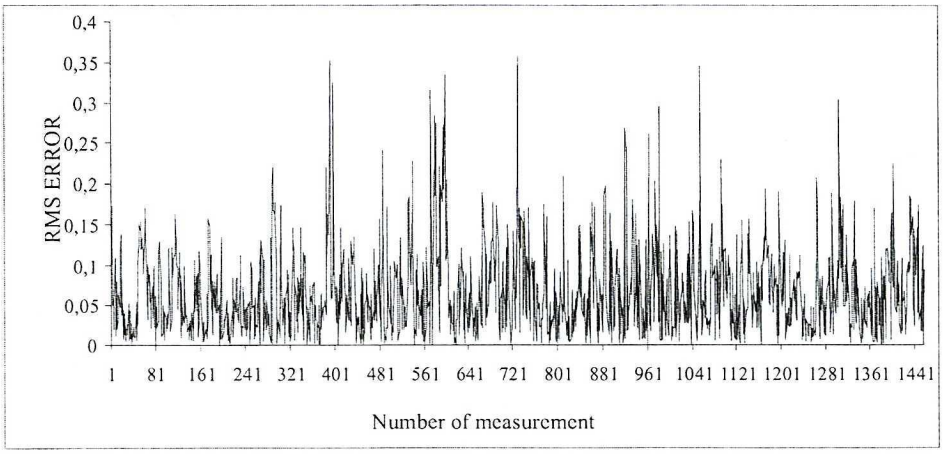

Fig. 10. RMS error for NO_2

greater sets of learning data containing base records with meteorological data and extreme values of concentrations.

However, it should be noted that the prediction was done by using the complete, finite set of measured data, presented to the network once at the stage of training. This way of running a network is natural in a case of its testing with already existing finite data set. The practical use of a network in concentration predictions would be related with somewhat different mode of proceeding. Namely, for each new prediction performed for presently possessed set of data the network should be trained by using the set used in the previous

training enlarged by recently received results. It would yield predictions a little worse than those received in the present work.

Apart from considering the network running and training methods and selecting of error functions, it should be said that ANNs, or more precisely MLPs, are applicable in predictions of air pollutants concentrations even within such areas as Gliwice, with numerous and hard to inventory pollution sources. Many papers confirm that ANNs are better than regression models or other statistical methods in predicting the concentrations [2, 7, 21, 26]. However, in the present paper the difficulties in modeling of emission fields, due to problems with prediction of extreme concentrations by neural models, are pointed out. It follows from the investigations and literature that the safest way for using ANNs should be limiting their use to predictions of concentrations up to and above admissible level, i.e. to ascertain exceeding of standards – exactly like Andretta did it in 2000 [1]. Such a division of air pollutant concentrations to be predicted ensures 90% accuracy as far as the data used in the present paper are considered.

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