THE NOx EMISSION ESTIMATION BY THE ARTIFICIAL NEURAL NETWORK: THE ANALYZE

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Abstract

The paper presents the preliminary investigations of nitric oxides (NOx) estimation from marine two-stroke engines. The Annex VI to Marpol Convention enforce to ship-owners necessity of periodical direct measurements of the NOx emission from the ship engines. It is very expensive procedure but with a low accuracy. Presented investigations show the possibility of estimation the NOx emission without direct measurements but using the artificial neural network (ANN). The paper presents method of choice the input data influenced on NOx emission and configuration of ANN and effects of calculations. The input data poses 15 parameters of engine working, influencing on NOx emission. The output data, necessary to learning the network, were NOx concentration in engine exhaust gases. We take into account two types of ANN; the 3-layer perceptron (MLP) with number of neurons in the hidden layer from 10 to 20 and the radial basis function neural network (RBF) with number of neurons in the hidden layer from 10 to 80. The input, validation and verification data was obtained from laboratory tests. After procedure of network configuration, the chosen ANN was learned by back propagation method. During this operation the weights of neurons were changed to minimize the root mean square error. We obtained ANN's, which allow us to estimate the NOx emission from laboratory engine with accuracy, comparable with Annex VI regulations.

Keywords: *emission, NOx, nitric oxides, ANN, Artificial Neural Network, perceptron, ship diesel engine*

1. Introduction

High toxicity of nitric oxides (NOx) contained in exhaust gases emitted from ship engines causes' high level of health hazard. To prevent of sea environment International Maritime Organization introduced Annex VI to MARPOL 73/78 convention in 1997. This Annex forces ship owners to limit NOx emission from the marine engines. The allowable level of this emission is defined in NOx Technical Code [1]. According to this Code, every introduced to operation onboard engines above 130 [kW] are obligated to have the valid certificate confirming the acceptable NOx emission. If marine engines are subjected some alterations during their operation period, they will have to extend such a certificate. Its prolonging consists in checking of a parameters and he structural parts of the engine influencing the NOx emission. Changes of engine structural parameters could entail the necessity of carrying out the direct onboard measurements of the NOx emission. Usually, the standard equipped engine rooms have not installed any appropriate analyzer of the exhaust gases. Therefore, such direct measurements lead to significant expenses for ship owners. Moreover, these measurements have to be carried out for strictly determined points of engine load. Such situation can also cause to withdrawing the ship with operation in order to perform these measurements, which are additionally not precise. According to the NOx Technical Code regulations, we can apply the simplified method during the onboard measurements. These regulations allow us to overcome the acceptable levels of emission even about 10% comparing with methods using on the shore. For the heavy fuel, these regulations allow to exceed this limit even up to 15%.

In order to make these regulations more applicable, many research centers work on alternative methods of NOx estimations from the onboard operated diesel engines. Kyrtatos et al. [1] proposes the „*software sensor for exhaust emissions estimation*“ based on multi-zone thermochemical model of NOx formation in the combustion chamber of the engine. This sensor includes only Zeldovicz's model [3] of NOx formation. Developing this method of NOx estimation the mono-zone multi-component, thermochemical model was proposed [4]. It's based on Konnov's model [5] and consists of 724 reactions between 83 chemical species. The conclusions formulated after researches on this model, show enough accuracy of NOx estimation only for one engine. Moreover, the complexity of NOx formation in the combustion chamber of the engine required very expensive computational power, not onboard accessible. The decrease of the modeling costs is possible by using the artificial neural network (ANN). Proposed by Werbos method of ANN learning [6], called the back propagation method, allows using the ANN in the various fields of knowledge. Wang et al. [7], Oladsine et al. [8] and Hafner et al. [9] uses ANN to control parameters of the piston engines and Stephan et al. [10] to control the power plant. Yang et al. [11] and Ramadhas et al. [12] proposes use ANNs to modeling of cetane number for blended fuels and Lee et al. [13] use ANN to modeling of the fuel spray penetration in the combustion chamber of the engine. The ANN was also applied to the lowering of the costs of the modeling of the combustion process reactions [14]-[18], specific fuel consumptions of the engine [19] and the temperature of the combustion process [20].

Presented works show, that using the ANN's is effective and not expensive alternative to the modeling of the combustion process parameters. According to this situation I would like to propose a method of the NOx estimation from the onboard diesel engine based on the measurements of working engine parameters like pressures, temperatures, etc. Moreover, I assume that these parameters measured in the standard equipped engine room are sufficient for developing the mentioned method. This, in turn, requires developing the appropriate model connecting these parameters into a function allowing for assessing a level of the NOx emission. In order to reduce the high cost of modeling the artificial neural network is proposed.

In this paper, the aspects of building and teaching the appropriate neural networks and some effects of NOx assessing was presented.

2. Formation of the NOx in combustion chamber of the engine

The main reason of NOx formation are a reactions of the nitrogen oxidization in environment of high temperature and high pressure in the combustion chamber. The nitrogen oxidized in these reactions comes from air and the fuel injected to the cylinder. The process of the nitrogen oxidation is reversible. Unfortunately, the quickness of reactions opposite to the oxidation is too low in the combustion chamber conditions. It causes to release some parts of the NOx to atmosphere during the scavenging process of the cylinder. Long-term investigations of the NOx formation carried out during the combustion process of a various flammable mixtures bring into being many mechanisms allowing for estimating the amount of the emitted NOx. Basing on thermal mechanism [21], we can state that the most important parameter of this process is its temperature. This statement is supported by results of experimental investigations presented in [22]. According to conclusions contained in [23], the second important parameter is pressure, causing for decreasing of NOx molar concentration. Investigations of Lyle and al. [24], shows us the considerable influence of relation between the molar concentration of the fuel and air on the NOx emission level. According to results of these studies, the prompt mechanism predominates in rich mixtures. After exceeding a stoichiometric air concentration in a mixture, the rapid growth of the NOx concentration occurs due to the thermal mechanism domination. However, the further increase of the air concentration causes for decreasing of the NOx concentration due to decreasing the combustion process temperature. Kuo [25] gives also dependences between the fuel composition and burning velocity, and the NOx concentration. According to results, a fuel molecular structure depends on burning the velocity and the NOx concentration, but this dependence is ambiguous.

According to these considerations the most important parameters influenced on NOx formation are:

- composition of burned mixture in the combustion chamber,
- time of combustion,
- pressure of combustion,
- temperature of combustion.

Values of these parameters are changed during the combustion process in the engine cylinder. Moreover, presented parameters couldn't be measured during sea operation of the engine. It means that estimation of the NOx emission requires measurement some another parameters of the engine working, influencing on temperature, pressure, time of combustion and composition of the combusted mixture. The author's research demonstrates [4], that measurement of the engine parameters during the sea operation conditions, are enough to the NOx emission estimation. The prediction of NOx emission by the direct calculation of NOx formation during combustion process is very expensive and difficult process [5], [26] - [28], requiring large computational power not attainable onboard. In this situation the direct calculation of the NOx formation to estimation of the level of the emission onboard is problematic. On the other hand properly learned neural network, may be sufficient tool to assess the level of the NOx emissions.

3. Artificial neural network preparing

According to the ANN theory [29] the enter data inserted to the ANN model has to comply appropriate requirements. The most important is the mutual independence of the enter data. It means that chosen entered data couldn't influence each other.

The earlier considerations show that the enter data to the ANN must represent the parameters influenced on NOx formation in the combustion chamber. The composition of the burned mixture in the combustion chamber may be estimated by the parameters of the air and the fuel at the inlet to the engine and the parameters of the injection system. We choose the following parameters: temperature and humidity of the scavenging air and a fuel consumption of the engine. Dependence between quantity of fuel and air in the combustion chamber is represented by an air/fuel equivalence ratio. Time of combustion is represented in enter data by speed of the engine and pressure of combustion is represented by the mean cylinder pressure, the maximum cylinder pressure and the crankshaft position at the maximum cylinder pressure. Temperature of the combustion process is represented in enter data by parameters of the injection process; the maximum injection pressure, the crankshaft position at the maximum injection pressure and temperature of the fuel before the injecting pump and temperature of the exhaust gas. The cooling system of the engine influences on temperature of the combustion process that has way the pressure and temperatures in the inlet and outlet of the cooling system were added to the enter data. According to these considerations 15 independent parameters of the combustion process are taken like the enter data to ANN.

The problem of NOx emission estimation from the diesel engine is classified as a regressive problem. General two types of ANN may be used to solve this class of problems. The first, most popular, network is multilayer perceptron (MLP) and the second the radial basis function network (RBF). Both are tested to solve this problem.

Structures of the MLP and RBF networks are similar and show in Fig. 1. The network consists of three layers; the input layer, one or more hidden layers and the output layer. All layers consist of an array of neurons.

The MLP neuron converts the input signals to output by sum of product of input signals and its weights. The result is passed through an activation function.

$$y = f\left(\sum_{i=1}^{n} w_i x_i\right), \tag{1}$$

where:

f - a nonlinear function called activation function,
x - an input signal,
w - a weight of the input signal,
n - a number of input signals.

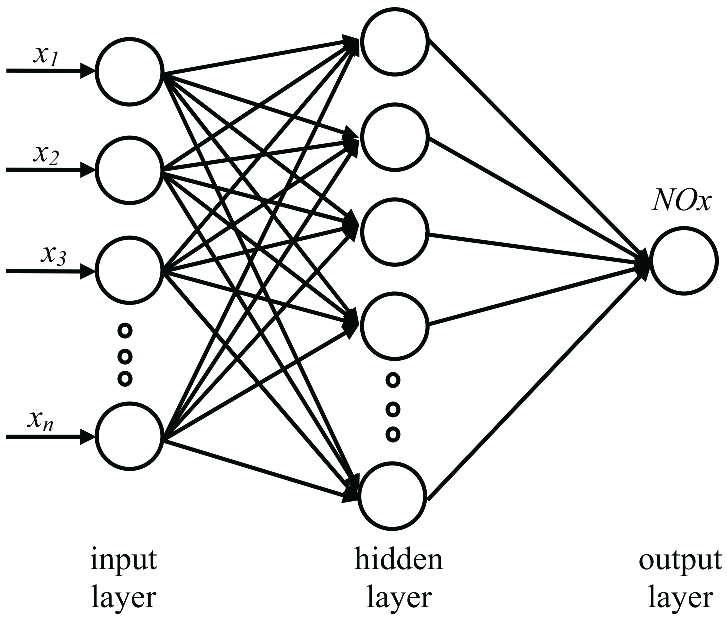

Fig. 1. The neural network structure

The RBF neuron contains a centre that is a parameter vector of the same dimension as the input signal and calculates the distance between the centre and the network input vector *x*. The result is passed through an activation function.

$$y = f\left(-\frac{\left\|x - c_i\right\|^2}{\sigma_i^2}\right), \tag{2}$$

where:

c - a centre of neuron,
σ - a positive scalar called a width of neuron.

During the investigations both, the MLP and RBF networks are considered. The networks consist of 15 input neurons in input layer for 15 enter data, one neuron in output layer for NOx emission estimation and neurons in one hidden layer. The number of neurons in the hidden layer was changed from 10 to 20 for MLP network and from 10 to 80 in RBF network. The input, validate and the test data were collected during the direct measurements on two stroke, one cylinder, loop scavenged, laboratory engine. The description of these investigations is presented in second part of this paper [30]. The 212 sets of data are collected after the measurements. The cross validation was used because of a small quantity of the data sets. In the model 162 data sets was randomly assigned as the data set, 20 to validation the networks, while the remaining 30 was employed for verification the performance of the ANN prediction. The logistic function as an activation function was used and the data sets before using were standardized to values from 0 to 1. The learning rate was set on 0,01.

The learning process for all considered ANNs consists of few stages:

- weights of all neurons were randomly assigned,
- inputs were presented to the input layer, and the output was calculated,
- weights were calculated by minimizing the error in back propagation process, this process was repeated to assign all data sets,
- data sets were mixed and the second epoch was started,
- after 200 epochs weights were calculated by minimizing the error in the conjugate gradient method by 500 epochs,
- the cross validation was used and repeated 5 times.

4. The results

The learning processes ANNs were prepared in STATISTICA 7.1 computer code. The root mean square errors for best ANNs after cross validation for all considered networks were presented in Fig. 2.

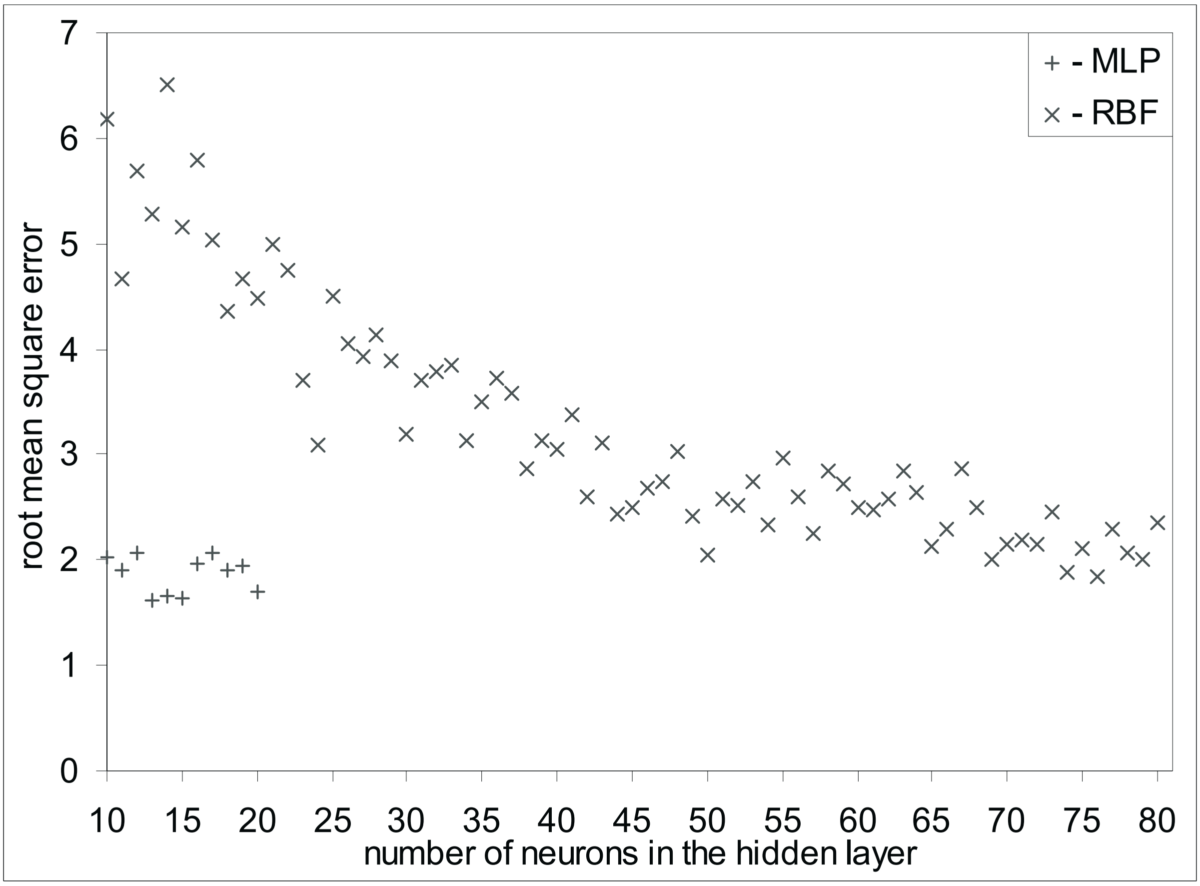

Fig. 2. The root mean square error for all considered ANNs

According to presented in Fig. 2 results, the MLP networks have littlest root mean square errors than RBF networks. Increasing of the number of neurons in the hidden layer cause decrease considered error. Increasing the number of neurons in the hidden layer of RBF network over 70 neurons decreases the error only imperceptibly. The changing of the neurons number in the MLP hidden layer between 10 and 20 neurons doesn't influence improvement of the quality of modeling significantly. The absolute value of mean error for all considered ANNs is presented in Fig. 3.

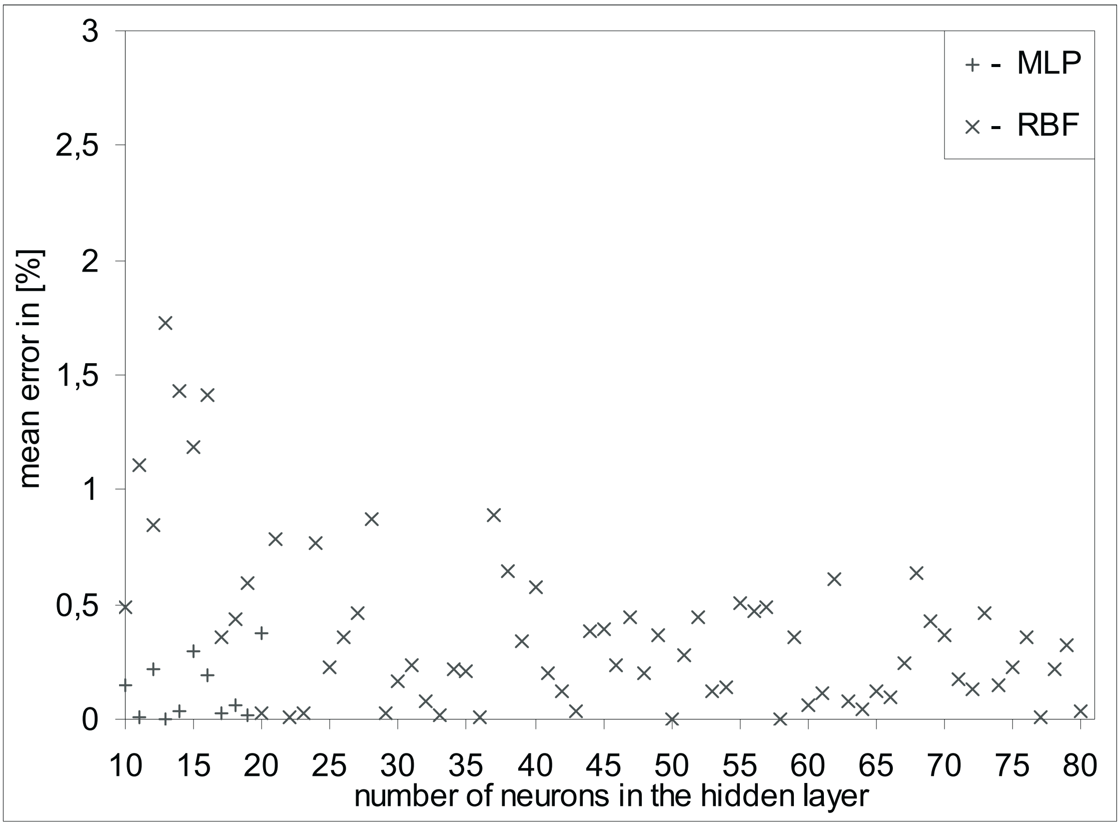

Fig. 3. The absolute values of the mean errors for all considered ANNs

According to results, presented in Fig. 3., all considered ANNs estimate the NOx emission in mean errors not excided than 1,75% for the RBF networks and 0,5% for the MLP networks but only few RBF networks have mean error excided 1%. According to these considerations the MLP networks are more usable to NOx emission estimation than the RBF network. The simplest configuration of the MLP network may to estimate the NOx emission from the marine diesel engine with better accuracy than the RBF network.

5. Conclusions

This paper describes the method of ANN preparing to the NOx emission estimation from the marine diesel engine during onboard operation. The presented results of this work enable the following conclusions to be drawn:

- the direct modeling of the NOx emission process from the marine diesel engine is difficult and expensive to onboard using,
- the preparing of the artificial neural network with considered enter data is sufficient to the NOx emission estimation from the marine diesel engine,
- increasing of the number of neurons in the hidden layer to improve the modeling accuracy is legitimate only for the RBF networks,
- increasing the number of neurons in the hidden layer of RBF network over 70 neurons decreases the error only imperceptibly,
- the simplest configuration of the MLP network may to estimate the NOx emission with better accuracy than the RBF network.

References

[1] *Interim Guidelines for the Application of the NOx Technical Code*, IMO News, No. 1, pp. 6, 2000.

[2] Kyrtatos, N. P., Dimopoulos, G. G., Theotokatos, G. P., Tzanos, E. I., Xiros, N. I., *NOx-box: A software sensor for real-time exhaust emissions estimation in marine engine,* Proceedings of IMAM 2002, Athens 2002.

[3] Heywood, J. B., Sher, E., *The Two-Stroke Cycle Engine. Its Development, Operation, and Design*, Taylor&Francis N.Y., 1999.

[4] Kowalski, J., Tarelko, W., *Nitric Oxides emission estimation based on measuring of work parameters of ship two-stroke engine*, Proceedings of 2nd International Conference on Marine Research and Transportation. Ischia Naples Italy,Session C, 2007.

[5] Konnov, A. A., *Development and validation of a detailed reaction mechanism for the combustion of small hydrocarbons*, 28-th Symposium (Int.) on Combustion. Abstr. Symp. Pap. p. 317. Edinburgh 2000.

[6] Werbos, P., *Beyond regression: New tools for prediction and analysis in the behavioural sciences,* Ph.D. Thesis, Harvard University 1974.

[7] Wang, W., Chirwa, E. C., Zhou, E., Holmes, K., Nwagboso, C., *Fuzzy neural ignition timing control for a natural gas fuelled spark ignition engine,* Proc. Instn. Mech. Engrs. Vol. 215, Part D, IMechE 2001.

[8] Oladsine, M., Bloch, G., Dovifaaz, X., *Neural modelling and control of a diesel engine with pollution constrains,* J. Intel. Robotic Systems, Vol. 41, Kluwer Academic Publishers, 2004,

[9] Hafner, M., Schuler, M., Nelles, O., Isermann, R., *Fast neural networks for diesel engine control design,* Control Engineering Practice, Vol. 8, Pergamon 2000.

[10] Stephan, V., Debes, K., Gross, H-M., Wintrich, F. Wintrich, H., *A new control scheme for combustion processes using reinforcement learning based on neural networks,* Int. J. Comput. Intel. Appl. Vol. 1, No. 2, Imperial College Press, 2001.

[11] Yang, H., Ring, Z., Briker, Y., McLean, N., Friesen, W., Fairbridge, C., *Neural network prediction of cetane number and density of diesel fuel from its chemical composition determined by LC and GC-MS,* Fuel Vol. 81, Elsevier, 2002.

[12] Ramadhas, A. S., Jayaraj, S., Muraleedharan, C., Padmakumari, K., *Artificial neural networks used for the prediction of the cetane number of biodiesel,* Renewable Energy Vol. 31, Elsevier, 2006.

[13] Lee, S. H., Howlett, R. J., Crua, C., Walters, S. D., *Fuzzy logic and neuro-fuzzy modelling of diesel spray penetration: A comparative study,* J. Intel. Fuz. Sys. Vol. 18, IOS Press, 2007.

[14] Blasco, J. A., Fueyo, N., Dopazo, C., Ballester, J., *Modelling the temporal evolution of a reduced combustion chemical system with an artificial neural network,* Combustion anf Flame, Vol. 113, Elsevier, 1998.

[15] Thompson, G. J., Atkinson, C. M., Clark, N. N., Long, T. W., Hanzevack, E., *Neutal network modelling of the emissions and performance of heavy-duty diesel engine,* Proc. Instn. Mech. Engrs. Vol. 214 Part D, IMechE, 2000.

[16] Cerri, G., Michelassi, V., Monacchia, S., Pica, S., *Kinetic combustion neural modelling integrated into computational fluid dynamics,* Proc. Instn. Mech. Engrs. Vol. 217 Part A, IMechE, 2003.

[17] Shenvi, N., Geremia, J. M., Rabitz, H., *Efficient chemical kinetic modelling through neural network maps,* Journal of Chemical Phisics Vol. 120, No. 21, American Institute of Physics, 2004.

[18] Kesgin, U., *Genetic algorithm and artificial neural network for engine optimisation of efficiency and NOx emission,* Fuel Vol. 83, Elsevier, 2004.

[19] Sayin, C., Ertunc, H. M., Hosoz, M., Kilicaslan, I., Canakci, M., *Performance and exhaust emissions of a gasoline engine using artificial neural network,* Applied Thermal Engineering Vol. 27, Elsevier, 2007,

[20] Parlak, A., Islamoglu, Y., Yasar, H., Egrisogut, A., *Application of artificial neural network to predict fuel consumption and temperature for a diesel engine,* Applied Thermal Engineering Vol. 26, Elsevier, 2006.

[21] Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill 1988.
[22] Bebara, L., Kermesa, V., Stehlika, P., Canekb, J., Oralc, J., *Low NOx burners-prediction of emissions concentration based on design, measurements and modeling,* Waste Management No. 22/2002, pp. 443-451, Elsevier Science Inc. 2002.
[23] Egolfopoulos, F. N., *Validation of nitrogen kinetics in high pressure fames,* Energy Conversion & Management No. 42/2001, pp. 21-34, Elsevier Science Inc. 2001.
[24] Lyle, K. H., Tseng, K. L., Gore, J. P., Laurendeau, N. M., *A study of pollutant emission characteristics of partially premixed turbulent jet flames,* Combustion and Flame No. 116/1999, pp. 627-639, Elsevier Science Inc. 1999.
[25] Kuo, K. K., *Principles of combustion,* Wiley. New Jersey 2005.
[26] Barlow, R. S., Karpetis, A. N., Frank, J. H., *Scalar profiles and no formation in laminar opposed-flow partially premixed methane/air flames,* Combustion and Flame No. 127/2001, pp. 2102-2118, Elsevier Science Inc. 2001.
[27] Bowman, C. T, Hanson, R. K., Gardiner, W. C., Lissianski, V., Frenklach, M., Goldenberg, M., Smith, G. P., Crosley, D. R., Golden, D. M., *GRI-Mech 2.11 An optimized detailed chemical reaction mechanism for methane combustion and NO formation and re-burning,* Topical Report Gas Research Institute 6/94-2/96.
[28] Curran, H. J., Gaffuri, P., Pitz, W. J., Westbrook, C. K., *A comprehensive modeling study of n-heptane oxidation,* Combustion and Flame No. 114/1998, pp. 149-177, Elsevier Science Inc. 1998.
[29] Masters, T., *Practical neural network recipes in C++,* Academic Press Inc., 1993.
[30] Kowalski, J., *The NOx emission estimation by artificial neural network: the results,* Journal of KONES, Vol. 15, Warsaw 2008.