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Determination of Nitromethane in the Air with the use of a Piezoelectric Sensors Set and Pattern Recognition Technique

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Abstract: To increase selectivity and sensitivity of determination of nitromethane in the air a set of piezoelectric gas sensors is proposed. In order to increase the differences between the signals sensor responses have been preliminary processed in accordance with the known algorithms. To determine nitrometane in the air an artificial neural network is applied and its parameters have been investigated.

Keywords: piezosensors, nitromethane, pattern recognition, artificial neural network

1. Introduction

An atmosphere is characterized by considerably spatial extension and a high rate of spreading of the local ejections of toxic substances as compared with the other natural objects (water, soil, flora). An effect of pollutants is determined by their individual properties and ability to interact with the other components contained in the air. Pollutants change the natural composition of the atmosphere thus resulting in appearance of danger for health of mankind and animals, facilitating destruction of environment and worsening conditions of work (unpleasant smells, low visibility).

In order to reduce detection limits of pollutants in the air it is necessary to elaborate new ways of their determination including selective ones. Contemporary approach to the detection of pollutants is tended to the application of fast-response sensors. Chemical and biological sensors are widely applied for analysis of the environment objects, industrial and medicine testing and control as well as for analysis of the foodstuff quality. Unlike of the standard methods (has chromatography, mass-spectrometry) specified sensors cannot solve such complicated problems [1]. The main problem is that they are insufficiently sensitive and they allow detecting only some classes of substances. Therefore, special systems have been elaborated, which use several sensors. The sensors work on the basis of one of the possible principles for transforming a signal (change of resistance, gas flow rate, capacity, quantity of work, mass, temperature or optical properties) [1,2]. There is a number of works on the qualitative and quantitative analysis with the use of a system of sensors and pattern recognition technique [1-8].

2. Experimental

Multi-sensor system has been applied for the determination of nitromethane. It was a set of sensors being in the same conditions with the following output of the analyzed signals to the register device and mathematical processing of the obtained data [1,2,7 – 10]. To analyze responses of a set of sensors an artificial neural network (ANN) [4,7] is applied. As compared with the other methods of pattern recognition ANN is able to:

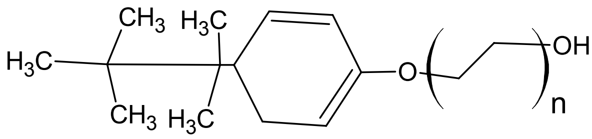
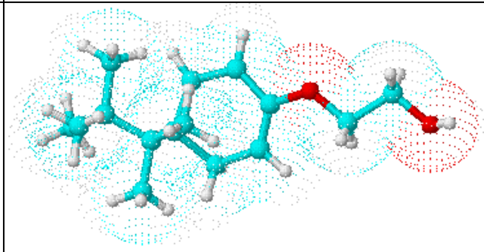
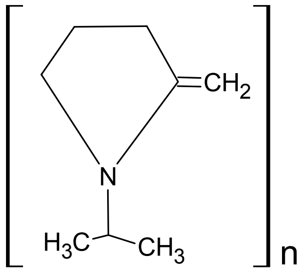
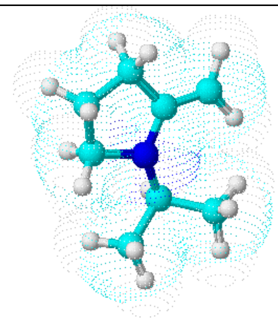
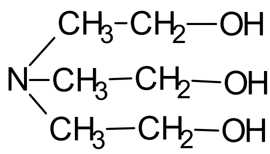
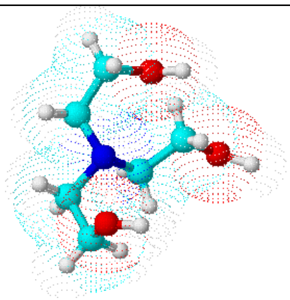
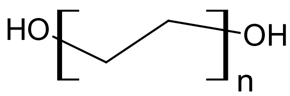
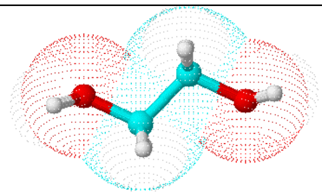
- – to be taught with a set of examples in case when there is no direct correlation between the input and output data;
- – to obtain results basing on incomplete, contradictory, noisy and distorted signal;
- – to process rapidly and with high efficiency a high data level and to follow hidden regularities;
- – to estimate comparative importance of the input information and minimize its amount without considerable losses of data.

After determining of the drift line and signal for each of a sensor optimization and learning of ANN are performed [4,7,10]. Then a number of latent neurons, an algorithm of preliminary input data preparation as well as norm and pulse of learning is varied in order to reduce an error of determination. Preliminary processing and pattern recognition algorithm are intended for realization of the hardware facilities allowing getting compact solution of localization for the analysis in the real time scale [1].

Piezosensors are rather simple to operate, small size and they can be applied for the determination of pollutants directly at the points of gas ejections. However, for the systems of complex composition their selectivity seems to be insufficient, extraneous components result in the considerable scattering of sensor response function from theoretical (mainly linear) dependence (Zauerbey equation) [18]. In order to obtain different selectivity and sensitivity relative to nitromethane sensors are modified with gas-chromatographic materials [19,20] (Table 1). Each of the sensors is sustained up to stabilization of its response. Efficiency of the operation of the artificial neural network depends on the signals received from a set of piezoquartz microbalances possessing specific responses. Therefore, it is necessary to maximize differences between the responses. To make this let us apply the corresponding algorithm of preliminary data processing. System response to the influence of nitromethane vapours in a wide range of concentrations of 0.005 – 0.075 g/m^3 has been investigated including maximum permissible concentration of nitromethane in the working area equal to 0.03 g/m^3 [21].

Neural network forming human brain is high-efficient, complex, non-linear system of the information processing [22]. It is able to organize neurons for perception of the pattern, its recognition or control of its motion much more rapidly than the comprehensive computers [23].

Table 1. *Modificators of Piezosensors.*

Modifiers	The chemical structure	The spatial structure
Triton X-100		
Polyvynil – pyrrolidone		
Triethanolamine		
Carbowax 20 M		

3. Results and Discussion

ANN form a simplified model of the brain and it is constructed on the basis of artificial neurons possessing the main property just as organic neurons – plasticity. The use of brain structure and neuron plasticity makes ANN a universal system for processing of the information. In general, ANN is an intelligent machine simulating brain operation. ANN realizes its computing power due to its two main properties – distributed in parallel structure and capability to learn and to extend the obtained knowledge. Extension of the knowledge means ANN ability to generate correct output signals for the input ones, which are not taken into account during the process of learning (training). Both of these properties make ANN a system for processing of the information that can solve complex multivariate problems, which are beyond the power for other methods of pattern recognition.

Neural network requires a special graduation procedure or learning in order to reduce the error of a model. A simplified algorithm of ANN learning with the use reverse error extension is constructed as follows:

1) One of the possible patterns is applied to the network input operating in the standard behaviour mode when signals are transmitted from inputs to outputs and then the values of sensor responses are calculated;
2) Next, ANN structure is corrected;
3) If network error is significantly large then one turns to step 1.

We have obtained experimental data in the form of a set of vectors (sensor responses to certain concentrations of nitromethane). To obtain the errors of determination sum of squares for the differences (SSD) between the output (O_j) and corresponding test values of the network signals (T_j) has been applied summarized over all the experiments:

$$SSD = \sum_{k=1}^{M} \sum_{j=1}^{N} (T_{jk} - O_{jk})^2 \quad (1)$$

where M is a number of experiments, N is a number of units for output data [1].

ANN structure (4:H:1, Figure 1) stipulated by its application for the determination of nitromethane concentration in the air. A set of 4 piezoelectric sensors is used; H is a number of neurons in the buried layer; these neurons realize non-linear input-output transformations of any degree of complexity.

Neurons of the input layer in the network transmit input signals to the first buried layer without their transformation. Next, non-linear transformation of signals proceeds consequently (layer by layer) in the buried neurons. Signals from the last buried layer are transmitted to the neurons of the output layer which form network response.

To minimize an error of nitromethane determination a learning algorithm for neural network has been applied called as “error backpropagation with impulse” [1]. Under controlled learning synaptic weights of ANN are adjusted for the approximating of the output data stored in the presenting practice patterns. After finishing of the learning procedure the network stores all the practice data and correctly responds to the test input signals. Beside an ability to store data this network can extend practice data.

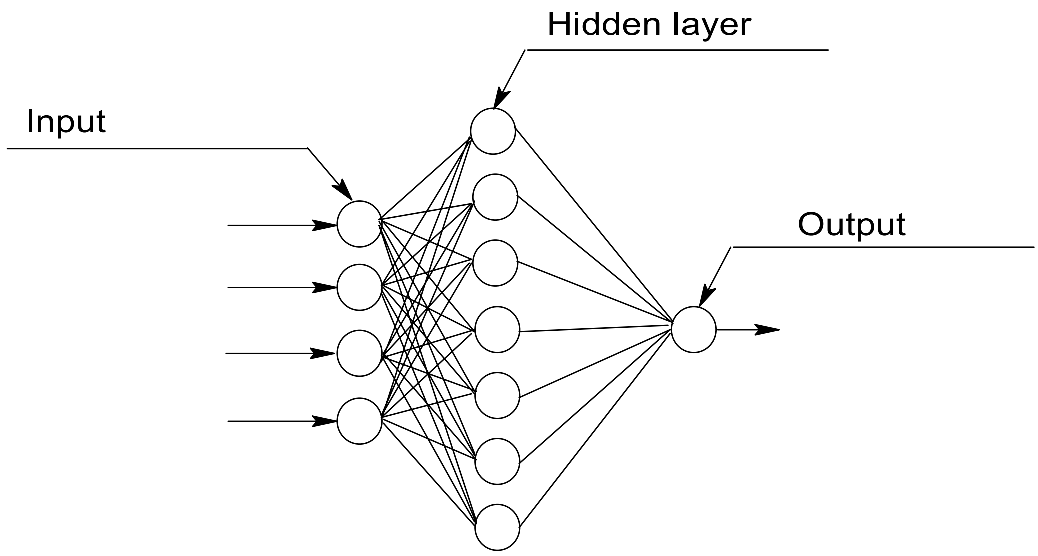


Fig. 1. *Artificial Neural Network Structure.*

Just as their biological prototypes ANN can learn – that means to improve their operation under the effect of environment changing ANN parameters. In the process of learning free parameters of neural network are adopted as a result of its continuous stimulation by the environment [24].

Figure 2 represents the learning scheme of ANN. A "teacher" has a base of knowledge about environment presented in the form of a set of samples input-output (database). A couple of these samples is called a practice pattern (example) which includes the input and output prototypes. A set of data couples represents a practice assembly of the patterns. At the first moment ANN does not possess any knowledge. In the process of learning the "teacher" and the network is exposed to the effect of environment – practice signal coinciding with one of the input patterns is applied to the inputs of these both elements. The "teacher" informs about correct (desired) response to the applied effect and yields corresponding output pattern. Basing on the value of an error between the real and desired output signals of the network ANN operation is then adjusted according to a certain rule. Repeating this process for many times ANN is adjusted in such a way that it apprehends "teacher's" knowledge about environment.

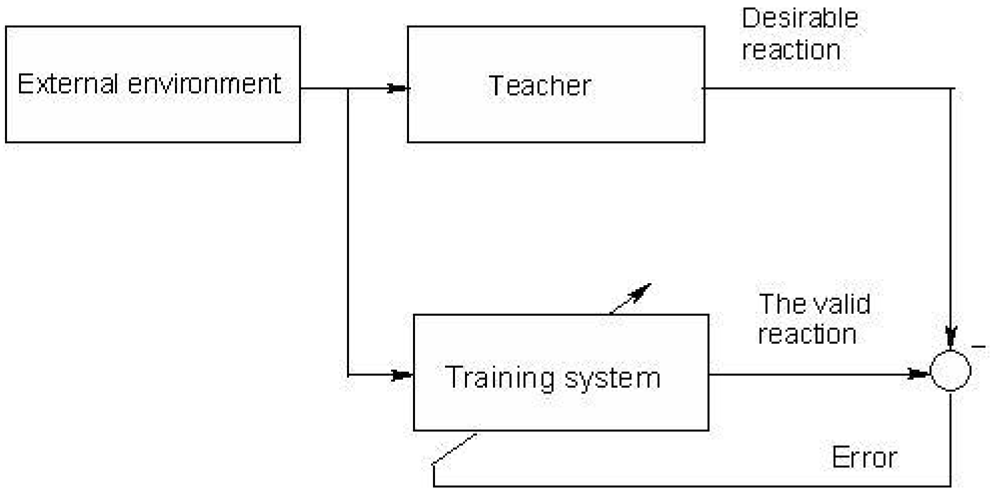


Fig. 2. *The Learning Scheme of Artificial Neural Network*

Algorithms for preliminary processing of the experimental data used for increasing of sensitivity and selectivity under determination of nitromethane by a system of sensors are presented in Table 2.

Table. 2. *Algorithms for preliminary processing of the experimental data*

Algorithms
F_{gas}/ F_{mod}
$(\lvert F_{gas} - F_{mod}\rvert)/F_{mod}$
$\lg(\lvert F_{gas}/F_{mod}\rvert)$
$\lg(\lvert F_{gas} - F_{mod}\rvert)/F_{mod}$

where F_{gas} and F_{mod} – piezosensor frequences before and after sorption, Hz; n – number of sensor controls in system.

To improve the work of ANN input data (sensor responses) have been arranged within relatively small interval lumped near zero for each algorithm [1]. Such scaling is described by the equation:

$$g_i^* = \frac{(g_i - \overline{g})}{S_i}, \qquad (2)$$

where g_i^* and g_i are scaled and non-scaled values of a signal of the *i*-th sensor, respectively; $\overline{g}$ and S are mean non-scaled value and standard scattering of a signal, respectively. Dependence in the change of determination error for different algorithms of preliminary processing of the experimental data is presented in Figure 3.

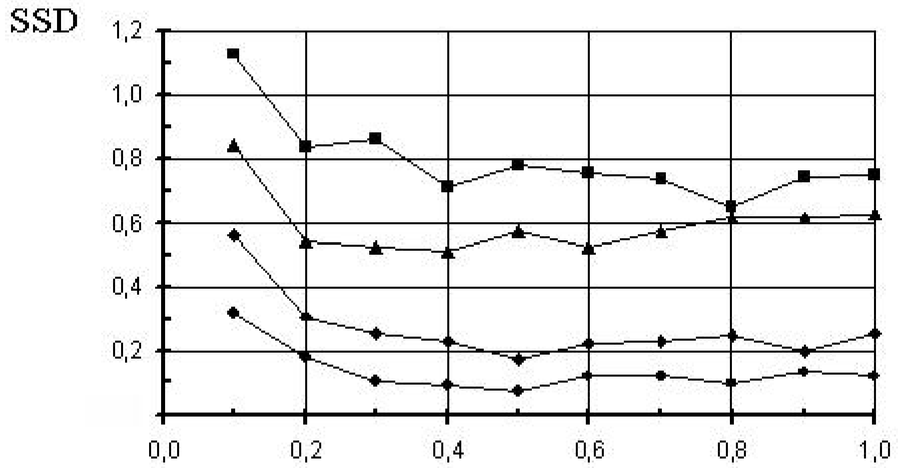


Fig. 3. *Change of Artificial Neural Network Error When Using Different Algorithms of Preliminary Processing of the Experimental Data.*

Influence of the number of neurons in the buried layer on the error of ANN has been studied (Figure 4). For more than 7 neurons in the buried layer an error of the network is not reduced. Thus, the optimum number of neurons in the buried layer is 7. Results of optimization of the neural network and its learning are as follows: - algorithm of preliminary processing is lg($|F_{gas} / F_{mod}|$); norm of learning is 0.1; pulse is 0.9; number of neurons in the buried layer is 7.

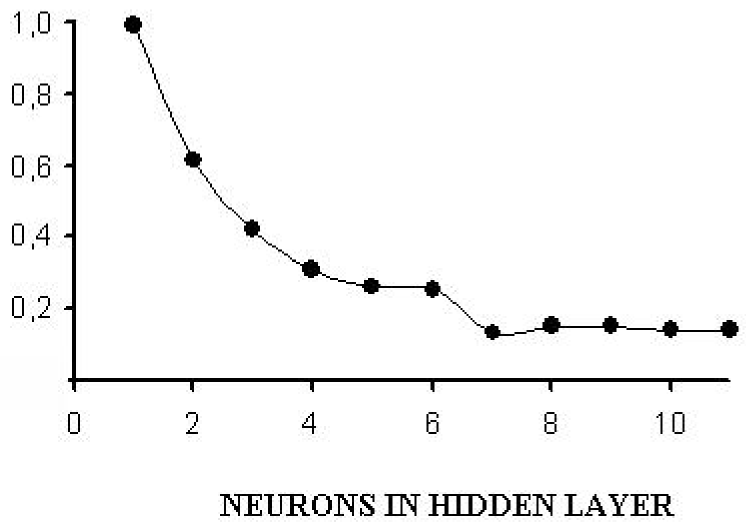


Fig. 4. *Influence of Neurons Number of in the Buried Layer on the Work of Artificial Neural Network*

In order to determine nitromethane concentration in the real time mode with the use of the elaborated system it is necessary to measure responses of a set of sensors and to present them in ANN. Fig. 5

demonstrates the results of determination of the real nitromethane concentrations in the air obtained after application of ANN.

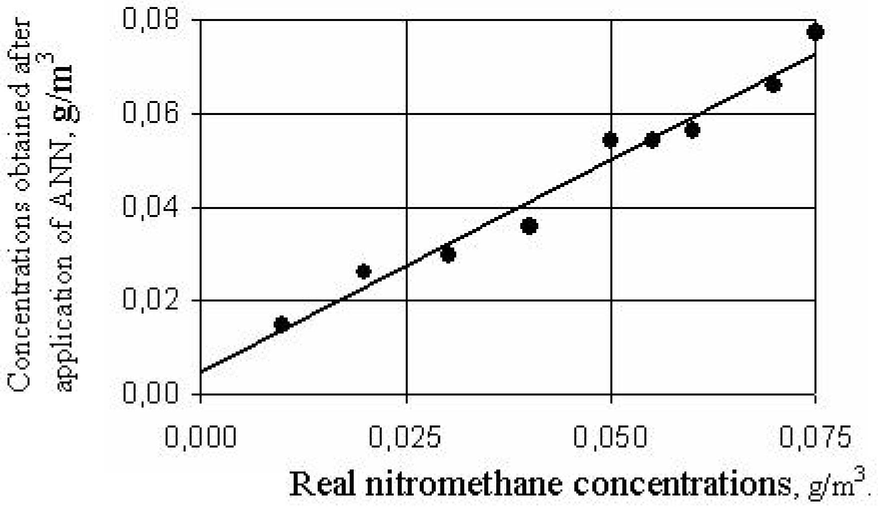


Fig. 5. *Prediction of Artificial Neural Network and Obtained Concentrations of Nitromethane.*

4. Conclusions

Responses of multi-sensor system to the exposure of nitromethane vapours in a wide range of concentrations (0.005 – 0.075 g/m^3) have been investigated; this interval includes maximum permissible concentration of nitromethane in the working area (0.03 g/m^3).

It is possible to make a precise determination of nitromethane concentrations in the air using a set of sensors composed of piezosensors. Responses from a set of sensors are applied to the input layer of artificial neural network. In order to reduce the error of determination the structure of ANN and its parameters have been optimized. Conditions of determination of nitromethane with the use of ANN have been found in the work: these are 7 neurons in the buried layer; impulse is 0.9; learning rate is 0.1; algorithm of preliminary processing is lg ($|F_{gas} / F_{mod}|$). A set of sensors is quite portable and it can be applied in the intelligence systems possessing abilities for independent estimation of the environment, detection of certain components, their recognition and instruction issue for corresponding execution units.

References

[1] Miguel M.A., Santos J.P., Agapito J.A. Application of artificial neural networks to calculate the partial gas concentrations in a mixture *Sensors and Actuators.* B 77 (2001). pp. 468 – 471.

[2] Gardner J.W. Detection of vapours and odours from a multisensor array using recognition. Part 1. Principal component and clyster analysis *Sensors and Actuators*. B 41 (1991). pp. 109 – 115.

[3] Lonergan M.C., Severin E.J. Array-based vapor-sensing using chemically sensitive carbon black-polymer resistors *Chem. Mater.* 8 (1996). pp. 2298– 2312.

[4] Sundgren H., Winquist F., Lukkari I. Artificial neural networks and gas sensor arrays: quantification of individual components in a gas mixture *Meas. Sci. Technol*. 2 (1991). pp. 464 – 469.

[5] Yang B., Carotta M.C., Faglia G. Quantification of H_2S and NO_2 using gas sensor arrays and an artificial neural network *Sensors and Actuators.* B 43 (1997). pp. 235– 238.

[6] White J., Dikinson T.A. Optical sensor array for odor recognition *Biosens. and Bioelectron*. 13 (1998). pp. 697 – 699.

[7] Endres H.E. A thin-film SnO_2 sensor system for simultaneous detection of CO and NO with neural signal evaluation *Sensors and Actuators*. B 35–36 (1996). pp. 353–357.

[8] Persaud K., Dodd G. Analysis of discrimination mechanisms in the mammalian olfactory system using a model system *Nature* 299 (1982). pp. 352 – 355.

[9] Gardner J.W., Bartlett P.N. Brief history of electronic noses *Sensors and Actuators* B 18–19 (1994). pp. 211 – 220.

[10] Gardner J.W., Bartlett P.N. *Electronic noses: Principles and applications*.–Oxford University Press, 1999.

[11] Gardner J.W., Bartlett P.N. Performance and standardization of electronic noses *Sensors and Actuators*. B 33 (1996). pp. 60 – 67.

[12] Shurmer H.V.An electronic nose – a sensitive and discriminating substitute for a mammalian olfactory system *IEEE Proc.– G. Circ. Dev. Syst*. 137 (1990). pp. 197–204.

[13] Gardner J.W., Hines E.L., Willdnson M. Application of artificial neural networks to an electronic olfactory system *Meas. Sci. Technol*. 1 (1990). pp. 446– 451.

[14] Axel R. The molecular logic smell *Sci. Am.* 273 (1995). pp. 154 – 159.

[15] Nagle H.T., Gutierez –Osuna R. The how and why of electronic noses *IEEE Spectrum.* 35 (9) (1998). pp. 22 – 34.

[16] Gopel W. Chemical imaging: concepts and vision for electronic and bio-electronic noses *Sensors and Actuators*. B 52 (1998). pp. 125 – 142.

[17] White J., Dikinson T.A. An olfactory neuronal network for vapor recognition in an artificial nose *Biol. Cybernetics*. 78 (1991). pp. 245 – 251.

[18] Malov V.V. *Piezoresonance sensors*. Moscow: Energoatomizdat, 1989.

[19] Pezev N., Kozev N. *The directory on gas chromatography*. Moscow: World, 1987.

[20] Lourier A.A. *Chromatographic materials*. Moscow: Khimiya, 1978.

[21] *Hazardous substances in industry*. Volume 2. Organic substances / Under red.. N.V. Lazarev.- Leningrad: Chemistry, 1976.

[22] Shepherd G. M., Koch C. Introduction to synaptic circuits *The Synaptic Organization of the Brain*. – New York: Oxford University Press, 1990.

[23] Churchland P. S. *Neurophilosophy: Toward a Unified Science of the Mind/Brain*. – Cambridge, MA: MIT Press, 1986.

[24] Mendel J. M., McLaren R. W. Reinforcement-learning control and pattern recognition systems. *Adaptive, Learning, Pattern Recognition Systems: Theory and Applications*. – New York: Academic Press, 1970.
