

## USING NEURAL NETS FOR REDUCING GAS CONCENTRATIONS BY THE DATA OF TRASS GAS ANALYZER AT CO<sub>2</sub>-LASER

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*Aspects of neural network construction and its learning for increasing accuracy of gas concentration reduction by measuring data of CO<sub>2</sub>-laser trass gas analyzer have been considered. Accuracy of reducing atmospheric gas (H<sub>2</sub>O, CO<sub>2</sub> и O<sub>3</sub>) concentration by neural network method in comparison with traditionally used method of least square is given.*

Trass gas analyzer on the basis of CO<sub>2</sub>-laser for concentration analysis of air composition has applied for a long time for research and environmental aims [1–5] and allows recovering mean value of studied gas (or gases) concentration along probing trass. Traditionally, the least-squares method (LSM) is applied for solving inverse problem [6, 7]. However, worst-case situations occur at the experiment, there are always errors of measurement of various nature that results in instability of solving the system of linear algebraic equation set. Instability appears either in negative or rather overrated values of recovered gas concentrations. Therefore, construction of more stable method of solving inverse problem is an actual problem. One of such approaches to inverse problem solution is the neural network method as we and other authors see it [8–14].

Intensity of the signal of trass gas analyzer on CO<sub>2</sub>-laser operating at wavelength may be written down as [1–7]:

$$I(v_i) = I_0(v_i) \cdot \eta(v_i) \times \exp\left\{-L \cdot \left(\sum_{j=1}^N k_j(v_i) \cdot x_j + \alpha_{aer}(v_i) + \alpha_{cont}(v_i)\right)\right\}, \quad (1)$$

where  $I_0(v_i)$  is the radiated intensity,  $L$  is the length of probing trass,  $k_j(v_i)$  is the attenuation coefficient of  $j$  gas for  $i$  wavelength,  $x_j$  is the concentration of  $j$  gas,  $\alpha_{aer}(v_i)$  is the aerosol extinction coefficient,  $\alpha_{cont}(v_i)$  is the coefficient of continuum absorption of water vapor,  $\eta(v_i)$  is the sensitivity of detector.

The procedure of recovering gas concentration depends on measuring circuit and may be fulfilled by the method of differential absorption (selection of sweep rate  $v_{ON}$ ,  $v_{OFF}$  – in absorption line (*ON*) and beyond it (*OFF*)) or sequential scan of atmosphere spectrum at selected rates of CO<sub>2</sub>-laser. Solution for the first measuring circuit consists in the fact that signals at rates  $v_{ON}$  and  $v_{OFF}$  are compared. The absorption coefficient of studied gas (or gases) may be found of the expression:

$$-\frac{1}{L} \cdot \ln\left(\frac{I(v_{ON})}{I(v_{OFF})}\right) - \Delta\alpha_{aer}(v_{ON}, v_{OFF}) - \Delta\alpha_{cont}(v_{ON}, v_{OFF}) = \sum_{j=1}^N \Delta k_j(v_{ON}, v_{OFF}) \cdot x_j, \quad (2)$$

where  $\Delta\alpha_{aer}(v_{ON}, v_{OFF})$ ,  $\Delta\alpha_{cont}(v_{ON}, v_{OFF})$ ,  $\Delta k_j(v_{ON}, v_{OFF})$  is the difference of coefficients of aerosol extinction, continuum absorption and gas absorption coefficients at rates  $v_{ON}$  and  $v_{OFF}$ .

Let us represent separate parts of the expression (2) in the form

$$\Delta y_j = -\frac{1}{L} \cdot \ln\left(\frac{I(v_{j,ON})}{I(v_{j,OFF})}\right) -$$

$$-\Delta\alpha_{aer}(v_{j,ON}, v_{j,OFF}) - \Delta\alpha_{cont}(v_{j,ON}, v_{j,OFF}),$$

where  $j$  is the number of pair  $v_{ON}$  and  $v_{OFF}$  for the investigated set of gases and matrix absorption coefficient difference  $\Delta K = K(v_{ON}) - K(v_{OFF})$ .

Then (2) is transformed to the matrix form:

$$\Delta y = \Delta K \cdot x. \quad (3)$$

Unknown vector of concentrations is found from the equation (3):

$$x = (\Delta K^T \Delta K)^{-1} \Delta K^T \Delta y. \quad (4)$$

Solution for the second measurement circuit is found from similar expression:

$$x = (K^T K)^{-1} K^T y. \quad (5)$$

Equations (3) may be solved as well by regularization method, then:

$$x = (K^T K + \alpha A)^{-1} K^T y, \quad (6)$$

where  $\alpha$  is the regularization parameter and  $I$  is the identity matrix.

Characteristics of accuracy of gas concentration recovery by the data of trass gas analyzer are examined in papers [6, 7], where it is shown that application of equations (4, 5) or (6) allows obtaining a good-enough solution up to the value of measurement error 15%. In some measuring cases the situations when solution can be achieved by none of circuits examined above occur. Besides, the solution depends significantly on selection of regularization parameter that makes find new parameter at change of measuring conditions. Therefore the modern and rather simple in computing respect method of neural network is suggested to be used for solving inverse problem.

The possibility of applying neural networks for solving inverse problem of recovering profile of ozone concentration in stratosphere by lidar data has been earlier examined. It was shown [15, 16] that neuronet technique does not yield in accuracy and rate to known approaches to inverse problem solution and exceeds them in safety. Using the results obtained before the method of neural networks is adapted to the task of processing the data of trass laser gas analyzer.

Neural network (NN) may be presented as a «black box» to the inputs of which the signals obtained at each rate of CO<sub>2</sub>-laser generation enter and the data of studied gas concentration are taken off the outputs. For the neural network developed in such a way to function and solve the assign task it should be trained (select learning algorithm as well as examples for learning that is pairs input-output connected with the formula (1) or obtained on the basis of natural experiment). After learning this method supposes introduction of model or measured signals to the NN input and obtaining of this or that gas concentration at the output.

Learning is an important stage; availability of the developed NN depends on its success. To calculate pairs of examples (signal – concentration) signals for different atmosphere states which are connected to the change of concentration range for each of studied gases were generated. The range of concentration change was selected on the basis of natural changes of studied gases in the air [17].

The learning methods of neural networks with a teacher may be divided into three large classes: stochastic, determinate and heuristic [14].

Stochastic learning method fulfills pseudorandom changes of weight values saving those changes which result in improving network operation results. Determinate learning method fulfills step by step the procedure of network weights correction based on use of their current values as well as input values (actual and desired yields). Genetic searching algorithm simulating processes of natural evolution and allowing selecting the best solution among the majority of solutions (populations) refers to heuristic learning algorithms.

The most used [12–14] approach to learning is in practice the determinate one for which various variants of algorithm of back propagation of error are developed. The known learning methods for stochastic approach are: Boltzmann machine and Cauchy machine. Choice between these approaches is determined as a rule by author preference or requirement of solved problem. There are no strict recommendations for definite selection of this or that approach. Therefore, it was decided to use several learning algorithms for comparing their functioning as well as selecting maximum efficient learning algorithm of neural network for solving this concrete problem.

Let us briefly examine these approaches:

#### 1. Modified method of back propagation of error.

Classical approach is based on the fact that gradient of network functioning error is computed for one example; network weighting factors are updated in direction opposite to gradient vector. In modified method it is suggested to give all examples, compute gradients then average gradient values and only after that update weights in direction opposite to average gradient.

#### 2. Genetic algorithm.

Genetic algorithm of minimum searching is based on simulating natural evolution process and refers to so called evolutionary search methods. Standard operations

changing solution are used at practical implementation of this method. Search for optimal solution is based on optimization of solution set.

To minimize the errors of neural network operation the algorithm of genetic search may be defined in the following way. A set of vectors of weighting factors – possible optimal solutions is determined. Each solution represents a chromosome and the availability function to the fact that solution may be left in sampling is calculated for each solution. Error function of network operation is usually used as such function. Solution set is called a population. Two or more solutions are selected of population and they are crossed into one forming a child. Crossing is a process of mixing chromosomes parents. It may be carried out by different methods; transferring one part of chromosome from one parent and another part of chromosome from another parent and so on and areas may be selected in different way.

The algorithm which in comparison with the known one allows using only a part of learning sample but not the whole one was developed for network learning on the basis of genetic algorithm.

Step 1. A number of copies of weighting factors (a number of individuals in population) is specified. Weighting factors in copies are filled with random values.

Step 2. The possibility of event of learning set change at insignificant distortion of sets is checked with low probability specified before. If this event has happened then the learning set is selected in a random manner. Summary error of learning is determined for each solution in population and it is written into learning error array of each individual. Summary error is determined from the equation

$$E_j = \sum_{i=1}^{NL} |f(x_{k,i}, w_j) - r_{k,i}|,$$

where  $NL$  is the number of examples in learning set,  $E_j$  is the summary error for  $j$  solution (individual) in population,  $x_{k,i}$  is the  $i$  input example of  $k$  set,  $w_j$  are the weighting factors of  $j$  solution,  $r_{k,i}$  is the output example,  $f$  is the result of network operation.

Step 3. Minimum value in error array is determined.

Step 4. Two solutions of population are selected for crossing for individuals with the smallest error.

Step 5. A child occurs after crossing two selected individuals. The pass is fulfilled at all network neurons, weighting factors in neuron are divided into two parts, point of divergence is selected in a random manner; weighting factors of the first parent are written into one part and ones from the second parents are written into second part.

Step 6. Mutation is carried out. Weighting factor is selected in a random manner. Then a random quantity is added to the value of weighting factor the maximum deviation of which is selected in a random manner from the array (1; 0,1; 0,01; 0,001)

Step 7. The error of the obtained solution is computed. If it is less than the maximum error in the error array then this individual is recorded instead of the most unadapted individual. Transfer to the Step 2.

### 3. Alternating-variable descent method.

The alternating-variable descent method is based on the fact that the search of network error minimum point starts from any initial point (random values of gas concentration from learning sample prepared beforehand). A step is made from the initial point along one of axes if error function decreases let us increase the step twice and made a step again if in this case the error increases let us decrease the step twice if error function does not decrease all the same let us make a step in other direction. If the error does not decrease any more and all possible directions are tested let us transfer to a new coordinate and make a step along the appropriate axis.

To implement the described approach to solving inverse problem of concentration analysis by the data of CO<sub>2</sub>-laser trass gas analyzer the software was developed on the basis of NN. It allows computing a signal of trass gas analyzer on the basis of equation (1) for the specified set of gases (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>, N<sub>2</sub>O, CH<sub>4</sub>, SO<sub>2</sub>, NO<sub>2</sub>, NH<sub>3</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>6</sub>H<sub>6</sub>) taking into account aerosol extinction and continuum absorption of H<sub>2</sub>O vapors. To simulate measurement errors the computed signal is distorted by a random number sensor.

The sequence of program operation is as follows: 1) one gas is selected from the list as a measured one, 2) the rest gases are taken into account and considered to be interfering, 3) the type of neural network is selected, 4) the neural network is trained and 5) the inverse problem solution directly for the model measuring conditions (for example, trass length, gas concentration, aerosol accounting) determined by a user. Processing of real signals of trass gas analyzer is possible on this stage.

When the studied gas is determined it is necessary to indicate the type of neural network. Adjusting neural network parameters it is necessary to determine a number of layers, quantity of neurons in a layer (Fig. 1), activating function type. Then one of the types of neural network learning (inverse distribution, genetic, alternating-variable descent or matrix) a number of examples of learning sample, a number of simultaneously used examples in one learning cycle and a size of test sampling (Fig. 1) are adjusted. Then the learning sample is generated and neural network type determined by a user is trained for the selected gas as a measured one. The

learning sample is constructed of size of changing of gas concentration according to [17] for the selected list of gases being a model atmospheric mixture. For example, for CO<sub>2</sub> surface concentration may vary during the day up to 10 % (in natural conditions) that is taken into account when determining concentration size of changing in learning sample for this gas. Selecting a large size of learning sample and slow learning a size of learning package may be adjusted some times smaller than a learning sample (let us call this part – package). This package is used in one cycle of neural network learning.

When all the parameters are adjusted the NN is learnt; learning errors are deduced individually for each gas. Appropriate NN parameters should be selected for achieving minimal learning error for each selected gas.

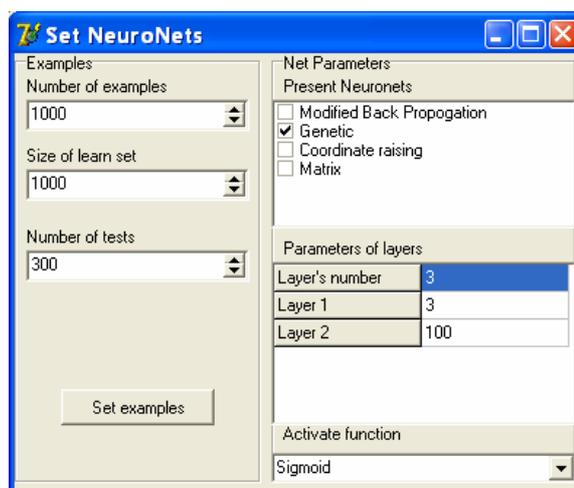


Fig. 1. Window for adjusting network parameters

On the basis of mass model computations of possibility of solving inverse problem of concentration analysis several algorithms of neural network learning were examined and genetic algorithm with sigma activation function seemed to be the most efficient (on the average minimum errors of gas recovery were achieved). To determine advantages and disadvantages of NN method solving the inverse problem it was compared with a less-squared method traditionally used in problems of concentration gas analysis. Simulation included three stages. On the first stage of program operation the atmosphere param-

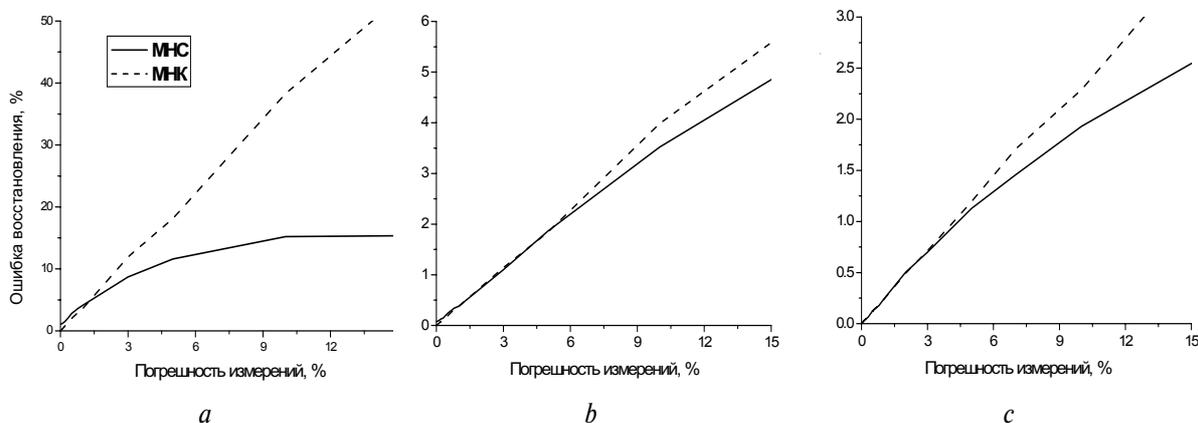


Fig. 2. Relative errors of recovering concentration of: a) O<sub>3</sub> b) CO<sub>2</sub> and c) H<sub>2</sub>O

ters (atmospheric gas model, aerosol model according to задавались [18]) neural network parameters (a number of layers: three layers, quantity of neurons in the layer: there are 3 neurons in the first layer, 100 neurons in the second layer and 1 output neuron in the third layer (value of studied gas concentration) were specified. On the second stage the network was learnt and on the third one the inverse problem was solved when model signals with different level of random noise simulating measurement errors were supplied to NN input.

The results of inverse problem solution for O<sub>3</sub>, CO<sub>2</sub> and H<sub>2</sub>O are given in Fig. 2. Diagrams showing relative error of ozone concentration recovery by the NN method (Fig. 3, *a*, carbon dioxide and Fig.3, *b*, water vapor) in comparison with the least-squares method are given in Fig 2, *a*.

It is seen from Fig. 2 that accuracy of gas concentration recovery is almost the same up to the measuring error of 3...5 %. Then at measuring error increase the accuracy of gas concentration recovery by the neural network method is higher. It appears clearer when recove-

ring ozone concentration that is conditioned by ozone low concentration (about 20 ppb) in surface layer of atmosphere. For gases which concentrations are rather high in atmosphere surface layer, for example, H<sub>2</sub>O (in summer it is about 1500 ppm) and CO<sub>2</sub> (about 330 ppm) solution of NN inverse problem differs slightly from traditional LSM (Fig. 2 *b*, *c*).

### Conclusion

Application of neural network method for solving inverse problem of concentration analysis by the data of measuring trass gas analyzer at CO<sub>2</sub>-laser has been examined. The results of solving inverse problem were compared with the traditionally applied least-squares method. It was shown that for some gases (H<sub>2</sub>O, CO<sub>2</sub>, O<sub>3</sub>) solution of inverse problem with neural networks at measuring error exceeding 5 % is more justified than application of the least-squares method. The results obtained in the article confirm the appropriateness of applying neural networks for solving inverse problem by the data of measuring with gas analyzer at CO<sub>2</sub>-laser.

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