# PARAMETRIC IDENTIFICATION FOR FOR MODEL OF A CHEMICAL HAZARDOUS SUBSTANCE CONCENTRATION USING SOFT COMPUTING

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***Abstract**: The technology of concentration determining for a hazardous chemical substance in the pre-accident period is suggested. As a concentration model was selected neuro-fuzzy network with fuzzy inference in Tsukamoto form. Parametric optimization of concentration model is proposed to carried out using a modified method of directional optimization. There are presents the results of numerical simulations.*

***Keywords**: Chemical hazardous substance, prediction, neuro-fuzzy networks, evolutionary modeling.*

***ACM Classification Keywords**: I.2.1 Applications and Expert Systems – Industrial Automation*

## Introduction

Last decade characterized by the development of information technologies as well as the growth of energy, metallurgy, chemical industry and agriculture, increased anthropogenic impact on the environment. Primarily it should be noted for the chemicals manufacturers and consumers. The increase in production volumes, competition and, consequently, decrease the rate of return, depreciation of fixed assets and investment flows behind the rate of depreciation is the cause of chemical accidents and disasters. Here are just some accidents of the last century and in recent years. In 1976 in Seveso (Italy) from the effects of chemical disaster affected more than 1,000 people, in 1978 in Suzhou (China) 3000 people were died, in 1984 in Bhopal (India) died 4035 people, in 1998 in Yaroslavl (Russia) in the affected area was more than 3,000 people, in 1989 in Jonava (Lithuania) spilled 7,000 tons of liquid ammonia, in 1991 in Mexico from the effects of chemical accident 17 people were died and 500 suffered, in 2010 in Hungary may be leaking tank of toxic waste and 10 people died, in 2012 in Latvia train derailed and 180 tons of chemicals spilled into the ground, in 2012 in Germany, there was a chemical accident with the release of chlorine and 39 people were affected, in 2007 in Ukraine was derailed train carrying yellow phosphorus, hundreds of people have been affected, in Gorlivka (Ukraine) in 2013 strait of ammonia occurred, five people died. The above are the most serious accidents, but their total number in the same period - tens or hundreds of thousands.

## Modeling of chemical accidents and its features

It would be premature to assume that in the near future the number of accidents decreased. Therefore, an important problem is to minimize their negative effects which primarily include the loss of life, environmental disasters and material damage. Its solution depends on the quality of decisions, as before the accident and after it. Information basis for this is the data on accident parameters, concentration of a chemical hazardous substance (CHS) and its dynamics in the infected area. This information allows in the pre-accident period to forecast and perform scenario analysis, and in post-accident - in time to evacuate people and carry out the correct actions.

As for chemical accidents natural experiment is not possible and they occur unexpectedly due to a confluence of circumstances, modeling plays an important role. Simulation allows you to get prior information about the possible flow and nature of the accident, its parameters and its possible consequences. The simulation results are not absolute, since any real chemical accident will be different from its simulated counterpart. However, the information obtained from the simulation is the basis for forecasting, determining the possible number of victims and material damage, the basis of decision-making processes.

It is important to note that an important role is played by a pre-accident modeling of the accident effects and post-accident simulation models to clarify the earlier results. At the same time, disaster simulation time should be as small as possible, because the scale of the consequences of accidents depends on the speed of decision-making and related activities.

The main objective of modeling is to determine the concentration of CHS as function of the accident parameters, the area coordinates, the time elapsed since the accident and the construction of the respective fields of concentration. This problem is solved in the pre-accident and post-accident period. What is the source of data for modeling? In most cases, the concentration is calculated based on known techniques. But the results have low accuracy, since the common techniques are focused on ideal conditions accidents running. It is difficult or even impossible to take into account the features of construction area and its topography.

An important feature of modeling is the impossibility of results verification. If by solution of other problems of identification and optimization exist the criteria for testing the effectiveness of the proposed methods, to calculate the accuracy of the method for determining the concentration CHS requires chemical accident that physically is impossible. Therefore, many authors to test the accuracy of their results using the results of experiments on the scattering of Freon-12 in an open space in the town of Thorney Island in the UK. To their description devoted entire issue of the Journal of Hazardous Materials [Journal, 1987]. These results will be used to verify the proposed technology.

To date, the most commonly used three approaches [Makhviladze, 2002; Shatalov, 2004] to the determination of the concentration of CHS based on the use of:

• Gaussian or dispersion models;

• scattering models, in which use integrated conservation laws in the cloud as a whole during burst release, here is included the model a "heavy gas";

• models of direct numerical simulation.

Each of these models has its particular applications, advantages and disadvantages. In particular, Gaussian models are based on heuristics to determine the factors that characterize the atmospheric instability. At the same time, the behavior at CHS emissions, especially near the point of release is much more complex than can be described by models of this type. It does not take into account the induced currents and the high density of the material. Earlier have been developed models that take into account relevant features of CHS ("heavy gas") and named scattering models "heavy gas". It is known implementation of such models: a methodology for the World Bank [Manual, 1988], HGGYSTEM [Hgsystem, 1994] proposed in ISO R12.3.047-98 [ISO, 1998], the method of RD 52.04.253-90 [RD, 1991]. A common drawback of these methods is inflated real consequences of accidents.

Another disadvantage of these models is their theoretical and practical low applicability as they are directed to use in post-accident period and are general in nature. At the same time, each chemical accident has specific features and determining concentration fields CHS using these models because of the large amount of computation and the need to specify the coefficients and parameters of the accident in critical conditions is the almost impossible problem.

## Models and Methods Structural and Parametric Identification

One way of solving this problem is the use of expert opinions based on experience, intuition, knowledge, results of the use of known techniques, the use of software to simulate the accidents effects, as well as climatic conditions and terrain. In such case it is necessary to determine the most likely area of infection, fiducials (the most typical characteristic of large areas) concentration point, the most possible parameters of possible accidents and form a table source data that contains database fields of the type:

$$BD_1 =< x_0,\ y_0, z_0,\ t_0, V,\ \nu,\ u,\ S >, \qquad BD =< x,\ y,\ z,\ t,\ C >, \tag{1}$$

where $(x_0, y_0, z_0)$ - the coordinate of the accident point, $t_0$ - the accident time, $V$ – an total emissions, $\nu$ - volume ejection speed, $u$ - wind speed, $S$ - the atmosphere stability by Pasqvill, $(x, y, z)$ - coordinate of the point in which in time $t$ the CHS concentration is equal to $C$ . The table containing the data (1), is the basis for model receive

$$C = F(x_0,\ y_0, z_0,\ t_0,\ V,\ \nu,\ u,\ S, x,\ y,\ z,\ t), \tag{2}$$

by which the field concentration can be obtained for any contamination zone at any time.

Obviously, the model (2) can be identified structurally and parametrically using different approaches and methods. The most common is to use multiple linear regression model [Gruber, 1996]

$$C = a_0 + a_1 X_1 + a_2 X_2 + \ldots + a_n X_n \tag{3}$$

as the solution of the structural identification problem and least squares method (LSM) as a method of parametric identification. Simplicity of this model is its advantage, but it is important to take into account that natural processes are essentially non-linear, and the use of the model (3) is relevant only to a small time or area intervals. Rational use of non-linear multiple regression model [Snytyuk, 2008]

$$C = a \cdot f_1(X_1) \cdot f_2(X_2) \cdot \ldots \cdot f_n(X_n), \tag{4}$$

where $f_i(X_i) = f_i(b_{i0}, b_{i1}, \ldots, b_{im_i}, X_i)$ - functions which by algebraic manipulation may be converted to linear models, $b_{j0}, b_{j1}, \ldots, b_{jm_i}$ - the parameters, $i = \overline{1,n}$ , $m_i$ - the number of parameters in the $i$ -th function. The advantage of this model is its non-linearity, but as the calculation of functions parameters carried out by LSM, it is necessary to check the conditions of its application. Furthermore, a function set is limited that indicate a disadvantage of a method.

One of the most accurate methods for approximate functions is the group method of data handling (GMDH) [Ivakhnenko, 1987]. The corresponding model is the Kolmogorov-Gabor polynomial

$$C = a_0 + \sum_i a_i X_i + \sum_i \sum_{j>i} a_{ij} X_i X_j + \ldots \tag{5}$$

The method works well on the "short" samples and limits the researcher only one of a finite set of support functions. It is quite difficult to implement, requires a considerable amount of computation. This result is very difficult to interpret.

Recently to identify tabulated dependencies using artificial neural networks (ANN) [Hickin, 2006]. It should be noted that the basic neural network architectures and training methods there are several dozen. The advantage of neural network identification is an almost complete absence of requirements to the original data. However, due to the problems of a local optimum, the network is in most cases very difficult to properly train, in addition, the result of its operation can not be interpreted.

Considering the application of these models and methods to solve the identification problem (2), we note that local solutions to their use in a limited and finite set of input data is available, but can not get a field of concentration. This conclusion is based on the inaccuracy of expert opinions, a small number of input data and a large number of parameters to be determined.

## Structural identification of CHS Concentration Model

Based on the above comments and observations as the model (2) is was proposed the use of fuzzy neural network as a technology that integrates the neural network advantages and its learning capabilities, the possibility of providing expert conclusions and its interpretations. One of the first fuzzy neural networks proposed Jang (J. - SR Jang) in 1993 [Jang, 1993]. This network is called ANFIS (Adaptive - Network - Based Inference System). Traditionally used in such a network fuzzy inference in Sugeno form. However, the consequent fuzzy production rules in Sugeno form is a weighted sum of the antecedent arguments, which for our problem is unacceptable. Therefore, it was suggested that a modification of ANFIS networks with fuzzy inference in Tsukamoto form [Snytyuk, 2008]. A speciality of this form is the monotony of consequent membership functions. Let the rules would be:

$P_1$: if $x_1 \in A_1$, and $x_2 \in B_1$, and $x_3 \in C_1$, then $y \in D_1$;

$P_2$: if $x_1 \in A_2$, and $x_2 \in B_2$, and $x_3 \in C_2$, then $y \in D_2$;

$P_3$: if $x_1 \in A_3$, and $x_2 \in B_3$, and $x_3 \in C_3$, then $y \in D_3$,

where $x_1, x_2, x_3$ - the input variables, $y$ - the resulting characteristic, $A_i, B_i, C_i, D_i$, - fuzzy sets with their membership functions, $i = \overline{1,3}$. A network of ANFIS is shown in Fig. 1.

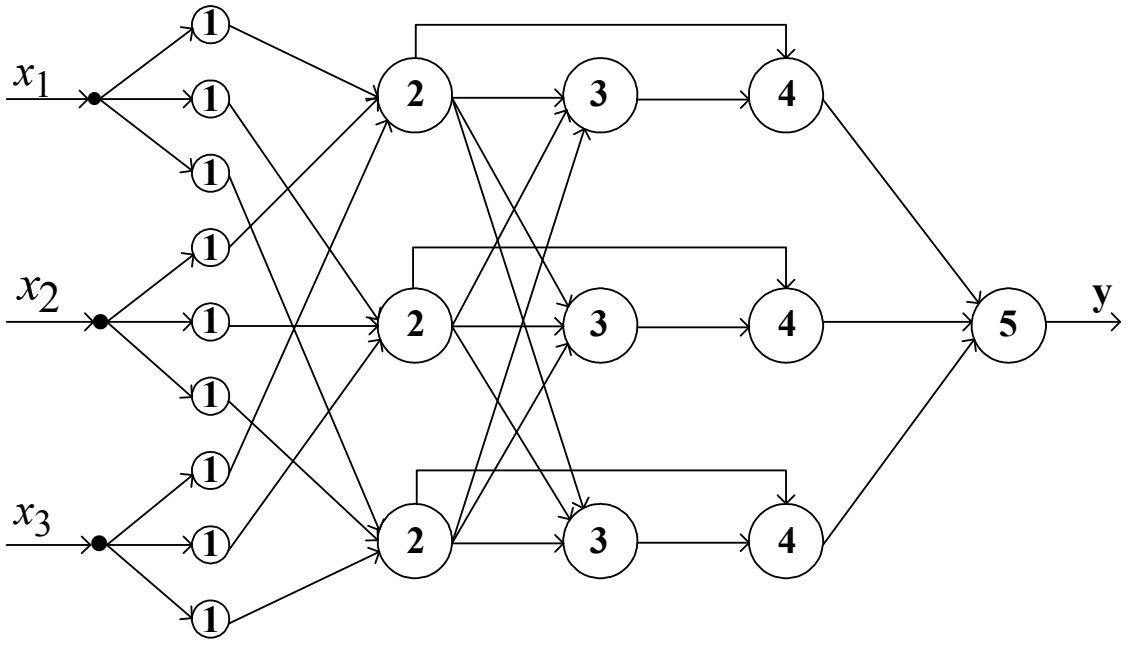


Fig. 1. ANFIS networks structure with fuzzy inference in Tsukamoto form

The input values of the network served In neurons of the first layer we find the values of membership functions

$$A_i(x_1^\circ), B_i(x_2^\circ), C_i(x_3^\circ),\ i = \overline{1,3}.$$

Thus, the number of neurons of the first layer (currently 9) coincides with the total power of set-term. In neurons of the second layer calculated values of truth measures for each rule from knowledge base:

$$\alpha_1 = A_1(x_1^\circ) \wedge B_1(x_2^\circ) \wedge C_1(x_3^\circ),$$
$$\alpha_2 = A_2(x_1^\circ) \wedge B_2(x_2^\circ) \wedge C_2(x_3^\circ),$$
$$\alpha_3 = A_3(x_1^\circ) \wedge B_3(x_2^\circ) \wedge C_3(x_3^\circ).$$

The number of neurons in this layer (there are 3) coincides with the number of rules. The same number of neurons contains the next layer and they calculated the relative importance of the rules:

$$\bar{\alpha}_1 = \frac{\alpha_1}{\alpha_1 + \alpha_2 + \alpha_3}, \quad \bar{\alpha}_2 = \frac{\alpha_2}{\alpha_1 + \alpha_2 + \alpha_3}, \quad \bar{\alpha}_3 = \frac{\alpha_3}{\alpha_1 + \alpha_2 + \alpha_3}.$$

Neurons in 4th layer perform operations

$$\bar{\alpha}_1 Z_1 = \bar{\alpha}_1 \cdot D_1^{-1}(x_1^\circ), \quad \bar{\alpha}_2 Z_2 = \bar{\alpha}_2 \cdot D_2^{-1}(x_2^\circ), \quad \bar{\alpha}_3 Z_3 = \bar{\alpha}_3 \cdot D_3^{-1}(x_3^\circ).$$

One neuron in last layer is assigned to find the sum:

$$y = \bar{\alpha}_1 Z_1 + \bar{\alpha}_2 Z_2 + \bar{\alpha}_3 Z_3.$$

As in the neurons of the first layer fuzzification is performed, it is necessary to know which of membership functions are carried out. Traditionally, learning neuro-fuzzy networks (NFN) is with using the gradient methods. This naturally requires that the membership functions are differentiable. Often are chosen a Gaussian or logistic functions. In real problems to train NFN using gradient methods is difficult and long, as each of the membership functions has, most often, two or three parameters. In the case of a large number of production rules to obtain an adequate result is almost impossible. So, if the number of input variables is ten, fifty the number of rules, the number of parameters will be several thousands. A tendency to converge the target function towards local optima does not allow for the training of NFN.

## Parametric Identification of CHS Concentration Model

Since the structure of NFN is already defined by production rules, it remains to carry out its parametric identification. Assume that all membership functions are the same type of Gaussian s $\mu(z) = \exp[-(z-a)^2 / 2\sigma^2]$ selected, where $a$ and $\sigma$ - the parameters. Then the number of parameters is equal to the product of the number of input variables on the number of rules, which are expert conclusions. If the conclusions are not equal or are made various experts, the number of parameters increases, as the importance of rules and the competence of the experts are parameters.

For parameter identification we choose the evolutionary algorithms. Such a choice is based on the fact that in this case there are no requirements for membership functions are differentiable and can avoid the problem of local optima. The traditional evolutionary algorithm has the following steps:

Step 1. In accordance with the required accuracy of the outcome to determine the set of potential solutions.

Step 2. Determine the sample population of solutions and to calculate the measure of optimality of each solution.

Step 3. While the algorithm stops condition is not satisfied to perform:

Step 3.1. Select solutions from the sample population.

Step 3.2. Implement crossover and select one of these solutions.

Step 3.3. With a certain probability mutate solutions.

Step 3.4. Record the decision in the new population.

Step 3.5. If the new population is not formed, then repeat steps 3.1-3.4. Step 4. End.

A potential solution to the problem of parametric identification is as follows:

$$z = (a_1, \sigma_1, a_2, \sigma_2, \ldots, a_m, \sigma_m, \xi), \tag{6}$$

where $m$ - the number of parameters of membership functions, $\xi$ - more options. The value of each parameter belongs to a bounded area defined by experts. There is therefore a need to test each potential solutions to its belonging to the area of possible solutions.

Any of evolutionary algorithms, which traditionally include genetic algorithms, evolutionary strategies, genetic programming and evolutionary programming requires a considerable amount of time for its execution due to unproductive search. So on with the parameter identification problem will be based on the use of well-known method EvoMax [Snytyuk, 2012].

## Adaptation of EvoMax to Parametric Identification of CHS Concentration Model

At the base of EvoMax is the idea to optimize random search of optimal solutions using evolutionary algorithms. This idea is based on the implementation of the targeted optimization using a composition of several techniques, in particular, elements of evolutionary strategies, the analytic hierarchy process and the elements of fuzzy sets theory. Let us consider a modified parameter identification method for determining concentration of CHS based on the EvoMax.

Traditionally EvoMax method is used to solve the problem of finding

$$\max_{X\in\Omega} f(X) \tag{7}$$

where $X=(x_1,x_2,\ldots,x_n)$, $\Omega$ - some hyperparallelepiped.

At the macro level, the proposed method will have the following steps:

Step 1. Number of iteration $e=1$.

Step 2. Determine the initial number of potential solutions $\lambda$ and generate uniformly distributed in $\Omega$ the potential solutions $z_1^e, z_2^e, \ldots, z_\lambda^e$, each of which has the form (6).

Step 3. We calculate the value of the function $f$ at the points $z_1^e, z_2^e, \ldots, z_\lambda^e$: $f_1^e = f(z_1^e), f_2^e = f(z_2^e), \ldots,$ $f_\lambda^e = f(z_\lambda^e)$.:.

Step 4. We normalize the values $f_j^e$ so $f_j^{ne} \in [0;1]$, $\sum_{i=1}^{\lambda} f_j^{ne} = 1$.

Step 5. Form the matrix of pairwise comparisons Saati $S$ so. Among the normalized values of the function we find the minimum $f_j^{ne}$, then divide the interval $[0;1]$ in 10 intervals: $[0;0,1),[0,1;0,2),\ldots,$ $[0,9;1]$. . Then for all $h\in\{1,2,\ldots,\lambda\}$, if $f_j^{ne}\in[0,1k;0,1+0,1k)$ and $f_h^{ne}\in[0,1l;0,1+0,1l)$ where $k,l\in\{0,1,\ldots,9\}$, then $s_{jh}=l-k+1$. Other elements of the matrix $S$ are calculated as follows: $s_{pq}=\frac{s_{jq}}{s_{jp}}$.

Step 6. We calculate the eigenvalues of the matrix $S$ and for the maximum eigenvalue $a_{\max}$ we find the corresponding eigenvector $w$. If the vector $w$ by a variety of reasons to find is problematic its elements are approximately calculated by the formula $w_j=\frac{1}{s_{1j}+s_{2j}+\ldots+s_{\lambda j}}$. Values $w_j$ indicate a measure of optimality (quasioptimality) potential solutions $z_j^e$.

Step 7. It is known [Rechenberg, 1994] that the next step should be the generation of "offspring" and the formation of a new population of potential solutions. The authors propose an evolutionary strategy to get "offsprings" as follows:

$$z_j^{e+1} = z_j^e + \xi(N(0,1)),\ j = \overline{1,\mu}, \tag{8}$$

where $\xi(N(0,1))$- a normally distributed random variable with zero mean and unit variance, $\eta$ - the number of "children" by one "parent". According to the concept of evolution by Charles Darwin $\mu > 1$, and in [Beyer, 2002] is recommended to choose $\mu \geq 7\lambda$. The last inequality is little conclusive.

We believe that to effectively finding of optimal solutions must be considered a measure of optimality $w_j$ for potential solutions $z_j^e$. It will allow only more detailed investigation of the area $\Omega$. Thus there are two hypotheses:

- if the value $w_j$ is the bigger, then the bigger should be the value $\sigma_j$ in generation of "offspring" of the potential solution $z_j^e$:

$$z_j^{e+1} = z_j^e + \xi(N(0,\sigma_j^e)), \tag{9}$$

which will expand the search area in the locality of a better solution, but in the least potentially optimal solutions will be the most narrowed area, including and because of its unpromising research;

- contrariwise, the bigger value $w_j$ is the cause of in-depth study of the most promising solutions locality and the bigger value will allow a detailed study of an area distant from the unpromising potential solutions.

These two hypotheses require confirmation, both of which are heuristic, but does not contradict the theory and practice of stochastic optimization. We bow to the correctness of the second hypothesis that is confirmed in the first experiments, but requires deeper investigation.

Another problem is to determine the optimal number “offsprings” depending on the solutions optimality. Obviously, this number $N(z_j^e)$ depends on the measure of area $\Omega$ and given accuracy $\varepsilon$ of the solution. For the case where $\Omega$ is a segment, $N(z_j^e) = g(L([a,b]))$, where $L(*)$ there is length. Determination of the value $\mu_j$ is also heuristic. In the first stage rationally believe that $\mu_j = \mu\ \ \forall i \in \{1,2,\ldots,\lambda\}$. Such conclusion is based on the second hypothesis and then for future solutions is necessary a deeper study of the locality, and for the unpromising - wider. And, both are equally important.

The most difficult is the problem of determining the variance value for each individual solutions. Obviously, $\sigma_j^2$ will depend, as in previous case, from $L([a,b])$, as well as the distance to the nearest neighbors solution. We find $d(z_j^e, z_L)$, $d(z_j^e, z_R)$ (the distance to the closest left (or point $a$) and right (or point $b$) of "neighbors" solutions). Suppose $d_{\max} = \max\{d(z_j^e, z_L), d(z_j^e, z_R)\}$, then $\sigma_j = \frac{1}{3} d_{\max}$, as by the well-known 3-sigma rule namely 10000 of 9973 points in the generation by the formula (8) belong to the interval $(x_j^e - 3\sigma_j, x_j^e + 3\sigma_j)$.

Step 8. In the previous step performed generate $\lambda \cdot \mu$ potential solutions. Find the corresponding values of the function $f$. From these values, and the values $f_1^e, f_2^e, \ldots, f_\lambda^e$ we determine the best $\lambda$ solutions $z_1^{e+1}, z_2^{e+1}, \ldots, z_\lambda^{e+1}$ and go to step 1.

Finding the optimal solution ends on $e$-th iteration when in step 2 $\max_{i,j}\left|f_i - f_j\right|$ will be less than some preassigned $\delta > 0$, so $\max_{i,j}\left|z_j^e - z_i^e\right| < \varepsilon$ that it shows the convergence of the method, $i, j = \overline{1,\lambda}$. Then, the solution $z_i^v$ which will correspond to the value $f_i^e = \max_j f_j^e$ will be a solution of the problem.

For the problem of parametric identification of CHS concentration model functions $f_j$ would be:

$$f_j = \sum_{k=1}^{p}(C_k - F(z_j, x_{0k}, y_{0k}, z_{0k}, t_{0k}, V_k, v_k, u_k, S_k, x_k, y_k, z_k, t_k))^2, \; j = \overline{1,\lambda},$$

and the problem (7) is transformed into the problem of finding

$$\min_e \max_{i,j}\left|f_i - f_j\right|, \; i, j = \overline{1,\lambda}.$$

Thus, for the structural identification of CHS concentration model is developed a model in the form of neuro-fuzzy network with logical conclusion in Tsukamoto form. For its parameter identification is proposed to use a modified method EvoMax for directed optimization.

## Experimental Verification of the Results

As mentioned above, the physical experiment for the problem is impossible, so we used the results of experiments on Torney Island. In these experiments reproduced huge emissions (exp. 07, 05, 08, 17) and a long release (exp. 45) freon-nitrogen mixtures in open space. The latter occurs when these initial data: emission volume 2000 m$^3$, the part in the gaseous mixture of Freon 31%, the wind speed 2 m/s, the stability of atmospheric by Pasquill was $E\left|F\right.$. In the huge emissions the gas volume was 2,000 m$^3$, the part of Freon in the gaseous mixture was 24%, the wind speed - 3.4 m/s, the stability of the atmosphere by Pasquill - E. These data were compared with predictions [Lisanov, 2005, Sumskoy, 2005], calculated for different techniques.

In order to forecast by the modified method EvoMaxM used expert conclusions, summarized in the table of type (1) having 54 lines. Seven lines of this table were used for the test sample. According to 47 conclusions was built neuro-fuzzy network and implemented its parametric optimization. Next, we calculated the value at a point on the axis along the direction of the wind at different distances from the accident point. The obtained values and the results of other methods for the experiment number 17 are shown in Table 1 and in Fig. 2. Comparison of the results is achieved by the mean relative deviation.

Table 1

Experience 17. Actual and predicted data for CHS concentration

| X,м | 40 | 50 | 70 | 100 | 140 | 220 | 500 | **mean relative** |
|---|---|---|---|---|---|---|---|---|
| C, % (об) | 12,1 | 8,4 | 4,7 | 3,1 | 1,35 | 0,6 | 0,32 | **deviation,%** |
| Phast | 11,2 | 9,5 | 7,5 | 4,2 | 2,4 | 0,95 | 0,18 | 23,43 |
| Toxi3 | 11 | 9,5 | 7,6 | 5,7 | 4,3 | 2,5 | 0,6 | 238,2 |
| Hgsystem | 3,8 | 3,1 | 2,2 | 1,5 | 1 | 0,5 | 0,2 | 23,62 |
| EvoMAxM | 12,2 | 7,9 | 4,1 | 2,5 | 1,4 | 0,72 | 0,21 | 4,24 |

Forecasting and comparative analysis were also carried out for other experiences. Application of EvoMaxM allowed us to obtain predicted values with the mean relative deviation within 2,2-6,3%, which was significantly better result compared with the results of other methods.

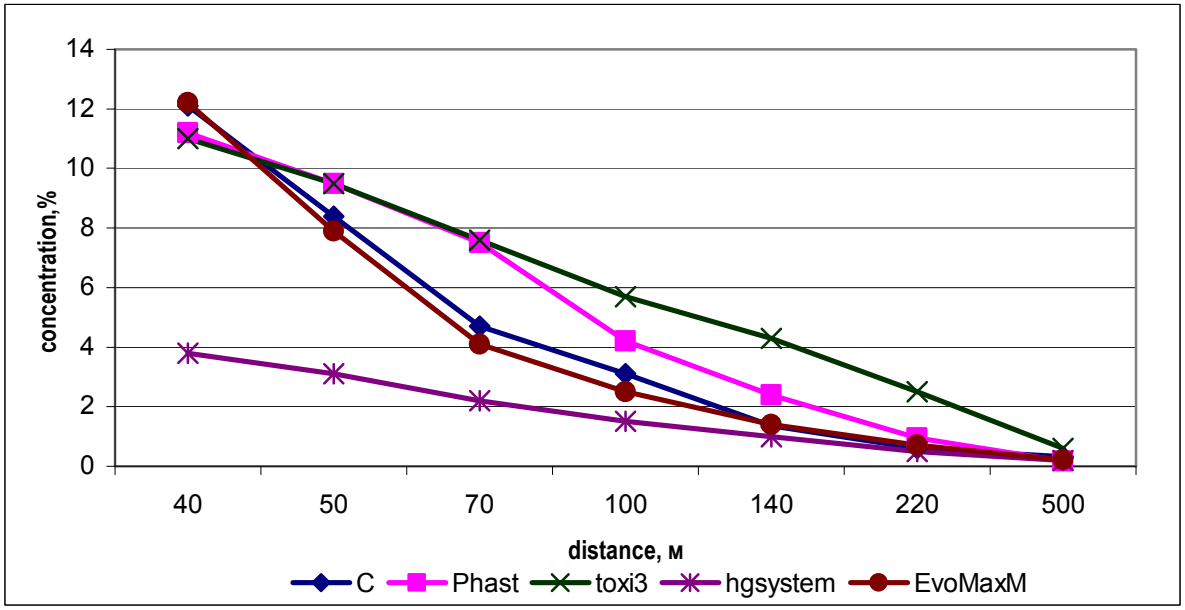


Fig. 2. Actual and predicted data for CHS concentration

## Conclusion and Perspectives

In this paper proposed a method for determining the CHS concentration in the pre-accident period. It is based on use of neuro-fuzzy network as a model, which allows the processing of expert conclusions and carry out further processing and interpretation of results. Optimization of network parameters based on the use of directed optimization EvoMax, as technology accelerated search for acceptable or quasi-optimal values.

The proposed technology can be used in the post-accident period to clarify the CHS concentration fields. Given the data point measurements of CHS concentration with instruments, neuro-fuzzy network can be retrained in the shortest possible time and be used to solve the problem of forecasting the CHS concentration in all possible contamination area. In addition, this technology can be used to refine the initial values of the accident parameters, that allow to improve and objectify decision-making processes.

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