

GEOECOLOGICAL MODELING THE ADSORPTION PURIFICATION OF POTABLE WATER

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Abstract

The complex modeling methodology of ecological systems and processes of water stream purification taking into account anthropogenic load, hydrodynamics and mass transfer in liquid and solid phases, forecasting with application of adsorption purification methods is offered.

Key words: *adsorption, purification, mass transfer, index of water pollution, environment*

Only complex geoecological modeling can adequately satisfy the requirements of nature management [1]. At the same time the vast majority of models do not fit in with the vast array of information in the descriptive natural sciences about the state of the natural environment in certain regions. Modeling is basically general, when information indicators for models require such indicators as the impact on the indexes of ecosystems quality assessment of mass transfer coefficient, diffusion, the degree of permeability and other characteristics. Obviously, such indicators and dependencies were not measured, are not measured and are not adequately monitored.

The system of sanitary and hygienic regulation with the use of MPC is subjected to a long-term reasoned criticism, since there has long been a tendency to assess the state of water bodies not from the point of view of the needs of a particular nature user but from the point of view of preserving the structure and functional characteristics of the whole ecosystem as a whole. Systematization of the main claims to the current MPC system is reduced to the following [2-7]:

- The concentration of substances in water does not reflect the toxicological load on the ecosystem, since it does not take into account the processes of accumulation of substances in biological objects and bottom sediments, i.e. the background associated with the accumulation of pollutants in the aquatic environment is not taken into account.
- MPC does not take into account the specifics of aquatic ecosystems the functioning in various natural and climatic zones and hence their toxic resistance.
- For justifying MPC the seasonal characteristics of natural factors are not taken into account against which the toxicity of pollutants is manifested.

The listed, as well as some other shortcomings of sanitary and hygienic regulation do not reject the need to assess the state of water bodies according to MPC but indicate the need to develop new approaches.

The main goal of both sanitary-hygienic and ecological rationing is to assess the quality class of aquatic ecosystems across the entire range of informative indicators. The importance of this problem is especially evident in the context of the sharply increased multicomponent nature of environmental pollution, when the main harmful factor is not the excessive normative concentration of harmful substances, but the complex "bouquet" of products synthesized in recent decades. For example, toxicology [8, 9] describes a syndrome of multiple chemical sensitivities that occurs as a result of the combined action of several chemical compounds at concentrations much lower than the thresholds of their harmfulness and manifesting in adaptation violation, loss of immunity, etc.

For justifying MPC, LIH - the limiting indicator of harmfulness for the most sensitive link is also installed at the same time. LIH is important in assessing the combined action of substances mixture. For example, if several chemical compounds belonging to the 1st and 2nd hazard classes are found in water and normalized for the same sign of harmfulness, it is necessary to determine the sum of the ratios of the actual concentrations C of each of them to the value of its MPC. As a result, this amount should not exceed 1 [10]:

$$\frac{C_1}{MPC_1} + \frac{C_2}{MPC_2} + \dots + \frac{C_n}{MPC_n} \leq 1 \quad (1)$$

The bottom accumulation coefficient (BAC) is defined as the ratio of the concentration of substances in the bottom sediments C_{bottom} to the concentration of the same substances in water C_{water} :

$$BAC = C_{\text{bottom}} / C_{\text{water}}. \quad (2)$$

The hydrochemical index of water pollution (IWP) was established by the State Committee for Hydrometeorology of the USSR [11] and belongs to the category of indicators most often used to assess the quality of water bodies (Appendix A). This index is a typical additive coefficient and represents the average percentage of exceeding of the MPC for a strictly limited number of individual ingredients:

$$IWP = \frac{1}{n} * \sum_{i=1}^n \frac{C_i}{MPC_i}, \quad (3)$$

where: C_i – concentration of the component (in some cases - the value of the physico-chemical parameter);

n – is the number of indicators used to calculate the index, $n = 6$;

MPC_i is the established value of the standard for the relevant type of water body.

When calculating the index of water pollution for the entire set of normalized components, including the pH value, the biological oxygen consumption BOC_5 and the dissolved oxygen content find the C_i / MPC_i ratios of the actual concentrations to the MPC and the found list is sorted.

Geocological modeling is one of the most important methods of scientific cognition of ecosystems with the help of which a model of the research object is created. Its essence lies in the fact that the relationship of the phenomena and factors studied is transmitted in the form of specific mathematical equations.

The process of constructing the geocological model includes the following typical stages: the formulation of modeling goals; a qualitative analysis of the ecosystem, based on these objectives; the formulation of laws and plausible hypotheses regarding the structure of the ecosystem, the mechanisms of its behavior in general or of individual parts; identification of the model; verification of the model (verification of its operability and assessment of the degree of adequacy to the real ecosystem); study of the model (analysis of the stability of its solutions, sensitivity to changes in parameters, etc.) and experiment with it.

For anthropogenic factors affecting the environment the term "contamination" is used to introduce materials or energy into the environment that can damage vital resources or ecological systems, or cause disturbances in their use [12].

The effect of an arbitrary factor of the environment X on any ecological indicator Y, which is taken as an assessment of the quality of the whole ecosystem, is traditionally described by some subset of mathematical formulas. The real instrumental measurement of many postulated parameters of ecosystems, first of all, specific parameters of material-energy, information flows between its elements, at the modern stage of development of science and technology is impossible. Usually only a limited set of factors that are often very indirectly related to the essence of the phenomenon under study is available to control or direct measurement.

In the synthesis of the ecosystem model we were interested in more generalized parameters such as the technogenic load on the reservoir, the influence of the hydrochemical pollution factors on such indicators as the hydrochemical index of water pollution (IWP), the ecotoxicological criterion according to T.I. Moiseenko X_{tox} , criterion W_{st} , taking into account the danger of sanitary-toxicological contamination, obtained for drinking water supply sources. These determining parameters of the ecosystem were calculated on the basis of model concepts of the process and were determined not by the error of the measuring device, which can be estimated at least theoretically accurately, but by the adequacy of the model used (equation, criterion, coefficient), i.e. the degree of approximation of the equation of the model describing the process to phenomena occurring in real nature.

The composition object characteristic matrices involved in the mathematical processing includes not only immediate values and factors of hydrochemical pollution - concentration C of contaminating components, the number of species of harmful substances, dissolved oxygen, biochemical oxygen demand, pH, coli index, but also obtained by us a set of adsorptive purification performance efficiency indicators - coefficient trapping substance by adsorbent bed ψ , the flow change of component picked up J_s , permeability coefficient of χ macromolecule of solute substances through the membrane pores, calculation of the concentration of the solute concentration in polarization C_0 area, calculation of ultrafiltration selectivity of the primary control parameters of process ϕ , concentration polarization factor k_p and others.

Consider the effect regularity of adsorption cleaning efficiency indicators and hydrochemical pollution factors on such indicators as the hydrochemical index of water pollution (IWP).

Mathcad 2001i Professional software was used to simulate the adsorption treatment of water. To calculate the dependencies of the ecosystem (Y) response to the environmental factors (X) we use the logarithmic functions Mathcad logfit (logarithmic), lnfit and lnfit (linear), pwrfit (power), genfit (generalized), lgsfit (logistic), expfit (exponential) to adjust the data and they correspond to the model. The calculated regression equations for the dependencies are presented in table 1.

Using the function logfit (logarithmic) Mathcad, which satisfies and adapts the data to the model function:

$$Y=a \cdot \ln(X+b)+c \quad (4)$$

we find the parameters of the function:

$$T=\text{logfit}(X,Y,G)$$

$$T=\begin{pmatrix} 0,504 \\ -4,926 \\ 5,468 \end{pmatrix}$$

Using these parameters and the range of variables to the graph $z=0...(X_n)$ we define the function $g(x)=T_0 \cdot \ln(x+T_1)+T_2$. We calculate the correlation coefficient $r=0,979$ and the determination coefficient $R^2=0,963$. At $r=0$ there is no linear relationship, and at $r < 0$ we are dealing with an inverse linear connection. The closer to 1 the value of R^2 , the better the quality of the model. When $R^2 \rightarrow 0$ two conclusions can be drawn: either the factor has no effect on the response, or the regression function is essentially nonlinear. Figure 1 shows the effect of the pollutant capture coefficient by the adsorbent layer K_c and the trapped component flow J on the IWP calculated from the model.

We define the function of the logarithmic model

$$Y=a\ln(X)+b, \quad (5)$$

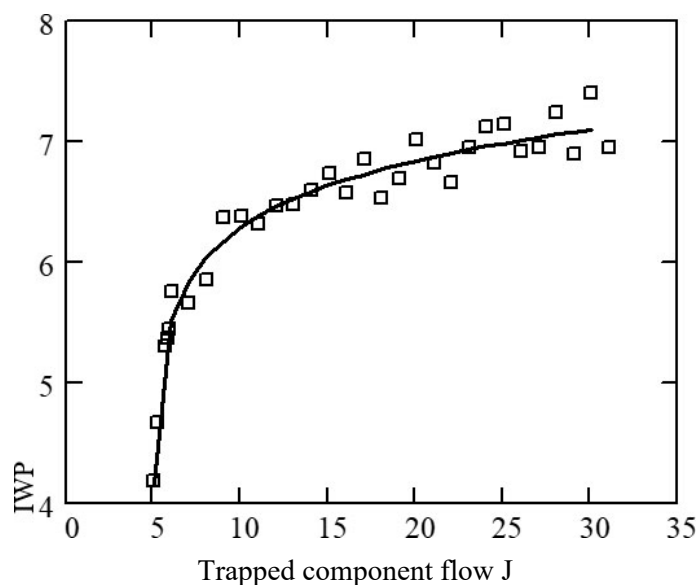
using function lnfit.

We use the function lnfit to find out the function parameters.

T:= lnfit (X,Y)

$$T = \begin{pmatrix} 1,168 \\ 3,312 \end{pmatrix}$$

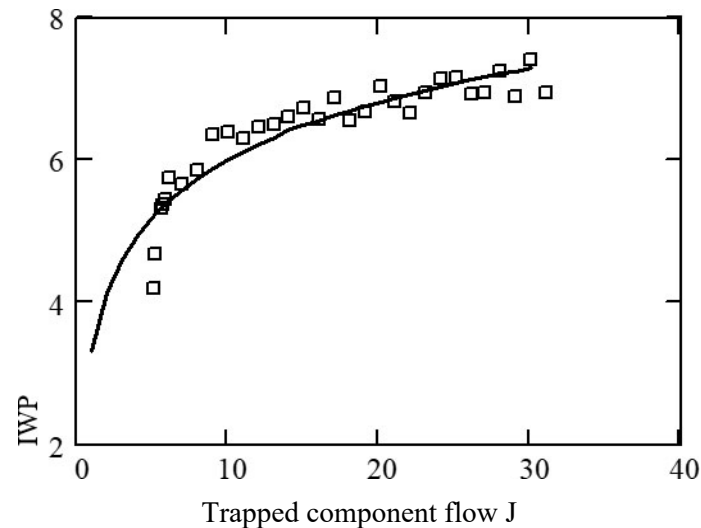
With variable ranges to the graph $z:=0...(X_n)$ we define the function $h(x):=T_0\ln(x)+T_1$. We calculate the correlation coefficient $r=0.921$ and the determination coefficient $R^2=0.848$. Figure 12 shows the effect of the pollutant capture coefficient by the adsorbent layer K_c and the trapped component flow J on the IWP by the logarithmic function.



Designations: points - experiment; line - calculation by model.

Figure 1 - Influence of the pollutant capture coefficient by the layer of adsorbent K_c and the stream J of the trapped component on the IWP

$$Y=a \cdot \ln(X+b)+c \text{ (logfit)}$$



Designations: points - experiment; line - calculation by model.

Figure 2 - Influence of the pollutant capture coefficient by the layer of adsorbent K_c and the stream J of the trapped component on the IWP

$$Y = a \ln(X) + b \text{ (lnfit)}$$

Now we use (Generalized) genfit, taking the function of the device:

$$Y = a X^b. \quad (6)$$

For this model, we define the function vector to use genfit.

$$F(n,a) = \begin{pmatrix} a_0 \cdot n^{a_1} \\ n^{a_1} \\ a_0 \cdot a_1 \cdot n^{a_1-1} \end{pmatrix}$$

We define the vector of assumptions.

$$\text{guess} = \begin{pmatrix} 1,5 \\ 0,5 \end{pmatrix}$$

Using genfit, we find the parameters in the function.

$$G = \text{genfit}(X,Y,\text{guess},F)$$

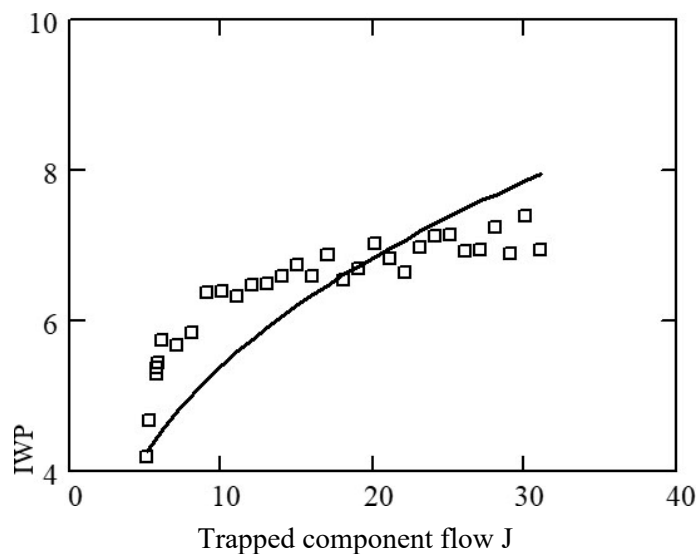
We find the values for the coefficients of the function.

$$G = \begin{pmatrix} 1,5 \\ 0,504 \end{pmatrix}$$

We define the function using these coefficients.

$$h(x) = G_0 x^{G_1}$$

Let us calculate the correlation coefficient $r=0.887$. Figure 3 shows the effect of the pollutant capture coefficient by the adsorbent layer K_c and the trapped component stream J on the IWP (Generalized) function.



Designations: points - experiment; line - calculation by model.

Figure 3 – Influence of the pollutant capture coefficient by the layer of adsorbent K_c and the stream J of the trapped component on the IWP

$$Y = a X^b \text{ (genfit)}$$

We use the logistic model (Logistic) lgsfit.

Function of the device:

$$Y = \frac{A}{1 + B \cdot e^{-C \cdot X}} \quad (7)$$

We define the vector of assumptions.

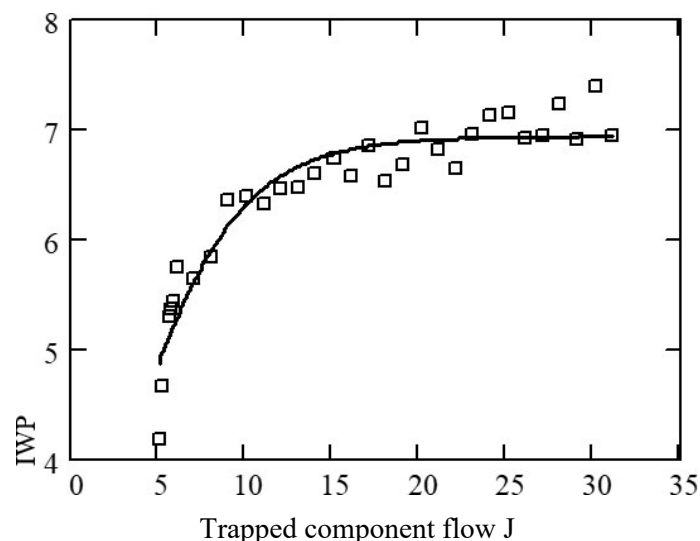
$$\text{guess} = \begin{pmatrix} a \\ b \\ -1 \end{pmatrix}$$

Find the values for the coefficients of the logistic function.

$$L = \text{lgsfit}(X, Y, \text{guess})$$

$$L = \begin{pmatrix} 6,934 \\ 1,809 \\ 0,291 \end{pmatrix}$$

Define the function $h(x) = \frac{L_0}{1 + L_1 \cdot e^{-L_2 \cdot X}}$, using these coefficients and the range of the variable to the graph $x = \min(X), \min(X)+0,1 \dots \max(X)$. We calculate the correlation coefficient $r=0.949$ and the coefficient of determination $R^2=0.9$. Figure 4 shows the effect of the pollutant capture coefficient by the adsorbent layer K_c and the trapped component stream J on the IWP by the logistic function.



Designations: points - experiment; line - calculation by model.

Figure 4 – Influence of the pollutant capture coefficient by the layer of adsorbent K_c and the stream J of the trapped component on the IWP

$$Y = \frac{A}{1 + B \cdot e^{-C \cdot X}} \quad (\text{lgsfit})$$

We use the regression (Power) pwrfit of the Mathcad to adjust the data to the model. Function of adaptation.

$$Y = aX^b + c. \quad (8)$$

We define the vector of assumptions.

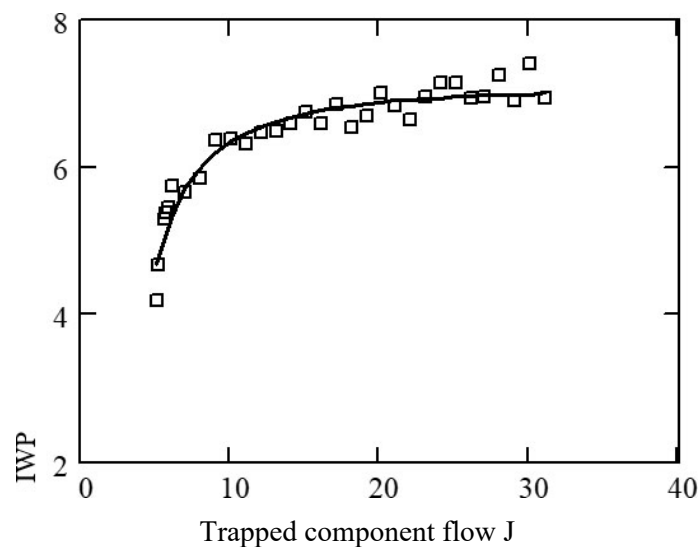
$$\text{Guess} = \begin{pmatrix} 2 \\ 0 \\ 0 \end{pmatrix}$$

We use pwrfit to find the parameters in the model function.

$$P = \text{pwrfit}(X, Y, \text{Guess})$$

$$P = \begin{pmatrix} 7,769 \\ 0,112 \\ -4,061 \end{pmatrix}$$

We define the function $H(x) = P_0 x^{P_1} + P_2$, using these coefficients and the range of the variable $x = \min(X) \dots \max(X)$ to the graph of the function. Let us calculate the correlation coefficient $r=0.914$. Figure 5 shows the effect of the pollutant capture coefficient by the adsorbent layer K_c and the trapped component flow J on the IWP on the function (Power) pwrfit.



Designations: points - experiment; line - calculation by model.

Figure 5 – Influence of the pollutant capture coefficient by the layer of adsorbent K_c and the stream J of the trapped component on the IWP

$$Y = a X^b + C \text{ (pwrfit)}$$

Table 1. Influence of environmental factors (X) on environmental indicators (Y) - indexes of water pollution (IWP).

№	Factor's name	Dependence	Function parameters	Coefficient of correlation r	Coefficient of determination R ²
On ecological indicator (Y) – index of water pollution (IWP)					
1	Pollutant capture coefficient by the layer of adsorbent K _c and the stream J _{Cg} of the trapped component on the IWP	$Y=a \cdot \ln(X+b)+c$	0,504 -4,926 5,468 (logfit)	0,979	0,963
2		$Y=a \ln(X)+b$	1,168 3,312 (lnfit)	0,921	0,848
3		$Y = aX^b+c$	7,769 0,112 -4,061 (pwrfit)	0,964	0,928
4		$Y = a X^b$	1,5 0,504 (genfit)	0,887	0,786
5		$Y = a \cdot e^{bX}$	5,278 0,011 (genfit)	0,83	0,689
6		$Y = a \cdot e^{bX} +c$	4,133 0,013 1,172 (expfit)	0,828	0,685
7		$Y = \frac{A}{1 + B \cdot e^{-C \cdot X}}$	6,934 1,809 0,291 (lgsfit)	0,949	0,9

Based on the results of calculations the following conclusions can be drawn. The function model in graph 1 with the found parameter values and the initial data points shows good suitability. The dependence $Y=a \cdot \ln(X+b)+c$ of the function logfit demonstrates a fairly close relationship between the flow of the trapped J_{Cg} component and IWP. The dependence $Y=a \ln(X)+b$ of the functions lnfit, linfit, and also $Y = a X^b$ genfit is significantly inferior to the statistical reliability criteria of equations 1 and 3 (Table 1).

The considered modeling methods allow to find the best functional dependence of the ecosystem response on the environmental factors. Moreover, the equation curve obtained as a result of processing the observational data allows us to understand the internal interrelations of the phenomenon under study.

REFERENCES

1. Abakumov V.A., Sushchenya L.M. (1991), *Hydrobiological monitoring of fresh water and the ways of its improvement. Ecological modifications and criteria of ecological regulation* [Gidrobiologicheskii monitoring presnykh vod i puti ego sovershenstvovaniya. Ekologicheskie modifikatsii i kriterii ekologicheskogo normirovaniya], Proceeding of international symposium, Gidrometeoizdat, Leningrad, 41-51pp.
2. Foroshchuk V.P. (1989), *Waterprotection activity and ecological regulation of water environment quality. Hydrobiological Journal* [Vodookhrannaya deyatel'nost' i ekologicheskoe normirovanie kachestva vodnoi sredy. Gidrobiologicheskii zhurnal], vol.25, No1, 36-41 p.
3. Khomyakov P.M., Ivanov V.D., Iskandaryan R.A. and others. (2002), *Geoecological modeling for environmental management purposes in condition of the change of natural environment and climate* [Geoekologicheskoe modelirovanie dlya tselei upravleniya prorodopol'zovaniem v usloviyakh izmenenii prorodnoi sredy i klimata], Moscow, 400 p.
4. Krasovskii G.N., Yegorova N.A. (2000), Hygiene and ecology criteria of harmfulness in the field of water body protection. Hygiene and sanitary [Gigienicheskiye i ekologicheskiye kriterii vrednosti v oblasti okhrany vodnykh ob'ektov. Gigiena i sanitariya], No6, 14-16 pp.
5. Luk'yanenko V.I. (1996), *Ecological MPC and integrated ecological monitoring of water quality. Rozenberg G.S., Krasnoshchekov G.P. Volga basin: ecological situation and ways of rational use of nature. Institute for Ecology of Volga Basin of Russian Academy of Science* [Ekologicheskie PDK i kompleksnyi ekologicheskii monitoring kachestva vod. Rezenberg G.S., Krasnoshchekov G.P. Volzhskii bassein: ekologicheskaya situatsiya i puti ratsional'nogo prorodopol'zovaniya. Institute ekologii volzhskogo basseina Rossiiskoi akademii nauk], Togliatti, 218-219 pp.
6. Manahan S.E. Environmental Chemistry. – NY.: Lewis Publish., 1994. – 789 p.
7. Methodical guidelines on integrated quality assessment of surface and marine waters. Approved State Committee of Hydrometeorology of UdSSR 22.09.1986 (1986), No250-1163, Moscow, 5 p.
8. Pykh Yu.A., Malkina-Pykh I.G. (1996), *About the assessment of environment state. Approaches to problem* [Ob otsenke sostoyaniya okrizhayushzhei sredy. Podkhody k probleme], Ecology, No5, 323-329 pp.
9. SanPiN 2.1.5.980-00 Sanitary rules and norms. Hygiene requirements to surface water protection (2000), Ministry of health of Russia, Moscow, 24 p.
10. Vorobeinik E.L., Sadykov O.F., Farafontov M.G. (1994), Ecological regulation of anthropogenic pollutions of surface ecosystem [Ekologicheskoe normirovanie tekhnogennykh zagryaznenii nazemnykh ekosistem], UIF Nauka, Yekaterinburg, 380p.
11. Zholdakova Z.I., Sinitsyna O.O., Kharchevnikova N.V., Zaitsev N.A. (1998), *Problem of united ecologic-hygiene regulation of chemical substances in environment. Hygiene and sanitary.* [Problema edinogo ekologo-gigienicheskogo normirovaniya khimicheskikh veshchestv v okruzhayushchei srede. Gigiena i sanitariya] No. 4, 57-60pp.
12. Zommer Ye.A. (1991), *Theoretical and experimental preconditions to development of ecological based regional MPC. Second Allunion conference on fishery toxicology. Proceeding* [Teoreticheskie i eksperimental'nye predposylki k razrabotke ekologicheskii obosnovannykh regionalnykh PDK. Vtoraya Vsesoyuznaya konferentsiya po rybokhozyaistvennoi toksikologii. Tez.dokladov], St.-Petersburg, 224-226 pp.