Modeling and Predicting the Organochlorine Pesticides Concentration in the Child's Body Based on their Accumulation in the Mother's Body

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Abstract. This paper describes the problem of developing a model of a polynomial neural network and applying it to predict the concentrations of organochlorine pesticides in a child's body on the basis of their accumulation in the mother's body. The results of the use of the developed models showed that the dependence of the concentration of organochlorine xenobiotics in the child's body on its concentration in the mother's body is non-monotonic. The developed models of the polynomial neural network allowed us to establish a critical interval at which an explosive transfer of persistent organochlorine xenobiotics takes place.

Keywords: Self-Organizing Modeling, Polynomial Neural Network, Model Validation, Organochlorine Pesticides, Persistent Organic Pollutants, Biomonitoring of Exposure Environmental Exposure, Pesticides Exposure.

1 Introduction

Environmental pollution by persistent organic pollutants (POPs) is one of the global environmental concerns. These compounds are very resistant to degradation processes, they have the ability to bioaccumulate and biomagnify, as a result of which they can accumulate in significant concentrations in the higher links of food chains even at low levels in the air, water, and soil. These features served as the basis for the fact that most of the organochlorine pesticides are classified as POP.

Environmental pollution with stable organochlorine pesticides (OCPs) is a serious environmental problem that is closely linked to health issues, as POP adversely affects the human body, having a toxic effect of a broad nature. The most sensitive indicator of assessing the health status of a population and the influence of environmental factors on it are indicators of the health of newborns, in particular, the prevalence of congenital malformations.

POP adversely affect human health, they cause changes in the neuroendocrine, immune systems, reproduction, and embryonic development. POPs affect the carrier's health, penetrate the placental barrier and significantly affect the course and outcome of pregnancy, fetal development and the health of the newborn, entering the baby's body as early as the neonatal period of development with the mother's blood and percutaneous fluid with amniotic fluid, in which xenobiotics enter breaking the placental barrier. Subsequently, the baby's load continues in the postnatal period: first, mainly with breast milk of the mother, and then - due to persistence and global prevalence in the environment with a diet. Changes in reproductive health indicators can sufficiently reflect the state of the environment, characterizing the mutagenicity and embryotoxicity of factors and their ability to suppress the adaptive mechanisms of the body.

OCPs enter the body of a child even in the neonatal period of development with maternal blood and percutaneously with the amniotic fluid, into which xenobiotics enter, overcoming the placental barrier. Subsequently, the effect on the baby continues in the postnatal period: first, mainly with breast milk of the mother, and then - due to persistence and global prevalence in the environment with a diet. Earlier, we conducted biomonitoring in the "mother - child" system.

Currently, it is believed that the detection of OCPs in food, air, and water, which are the main sources of their entry into the human body, is only evidence of its possible chemical exposure. At the same time, the results of biomonitoring of exposure (BME), that is, the identification and quantification of xenobiotics in human biological environments, is complete evidence of their presence and health risk [1-3]. Therefore, we conducted a screening with BME-resistant OCPs from among POPs, namely, those that were determined by us in environmental objects among the adult population and the children most vulnerable to their negative influence.

2 Problem Statement

The task is to simulate the effect of the content of γ hexachlorocyclohexane (HCH) and its isomers α and β on the composition of the whole blood of the mother and the blood of her child.

Formally, this problem can be considered as a class of tasks for modeling a statistical sample that contains information about n observations of m input variables. The statement of the problem of constructing models from experimental data can be reduced to searching for the extremum of a certain CR criterion on a variety of different models $\mathfrak{I}$:

$$f^* = \arg\min_{f \in \mathfrak{I}} CR(f) \quad (1)$$

It is clear that (1) does not contain a comprehensive formulation of the problem, so it is additionally necessary to: specify the type and amount of source information; specify the class of basic functions (operators) from which the set $\mathfrak{I}$ is formed; determine the method of generating models f together with a method for estimating parameters; choose a criterion for comparing models; indicate the CR minimization method. We refine this statement by assuming that the given sample $W = [Xy]$, contains n observation points, form the matrix $X = \{x_{ij},\ i=1,...,n;\ j=1,...,m\}$ and the vector $y = (y_1...y_m)^T$, so $n \geq m$.

3 Review of the Literature

The results of a study of invasive and non-invasive biological media of the mother (hair, whole venous blood, placenta, breast milk) and the baby (whole umbilical cord blood, which is considered the blood of the baby) indicate their multi pollution of OCPs and their derivatives. There are almost no examples of such complex studies, with the exception of [4,5]. They are of particular importance for identifying correlative relationships characterizing the processes of xenobiotic transfer from mother to child. The creation of a mathematical apparatus for their description is of great prognostic value for identifying risks to the health of a nascent child.

In [6], multivariable linear regression models were used to identify the relationship between the concentration of polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers (PBDEs), lead and mercury in maternal blood during pregnancy, and their content in umbilical cord blood.

In [7], using multiple regression analysis, the relationship between the Kinder Infants Development Scale (KIDS) and the levels of 3-phenoybenzoic acid, 3-PBA) of the maternal urethra was investigated.

In [8], the use of a neural network for determining the concentration of pesticides in maternal blood during pregnancy and in the umbilical cord blood of a child is described. The authors used a combined analysis of prenatal analyzes of mother's hair and blood, as well as neonatal tests such as hair, baby's blood, umbilical cord blood, and meconium to identify the effects of environmental pesticides on the fetus.

In [9], the concept of developing alternative tools for modelling toxicity and predicting chemical compounds was described in order to minimize animal tests, costs, and time associated with registration and risk assessment processes. The concept of multilevel self-organization for multidimensional modelling, as well as model verification, is proposed.In [10], a combined statistical analysis was proposed to identify the effects of environmental pesticides on the fetus.

Thus, the task of constructing mathematical models for the transmission of POP, and their metabolites from mother to child becomes relevant. In this paper, to solve the problem of predicting the transmission of POP and their metabolites from mother to child, GMDH neural networks are used. It is expected that the use of GMDH-neural networks will increase the efficiency of the developed model and maintain sufficient algorithm stability when working with various types of input information.

The purpose of this study is to obtain a model of a polynomial neural network that reproduces the level of chlorine-containing pesticides such as hexachlorocyclohexane and its isomers to their content in the body of a child of a particular mother.

4 Materials and Methods

In the general case, the process of constructing models from experimental data (1) includes, first of all, the following main stages:

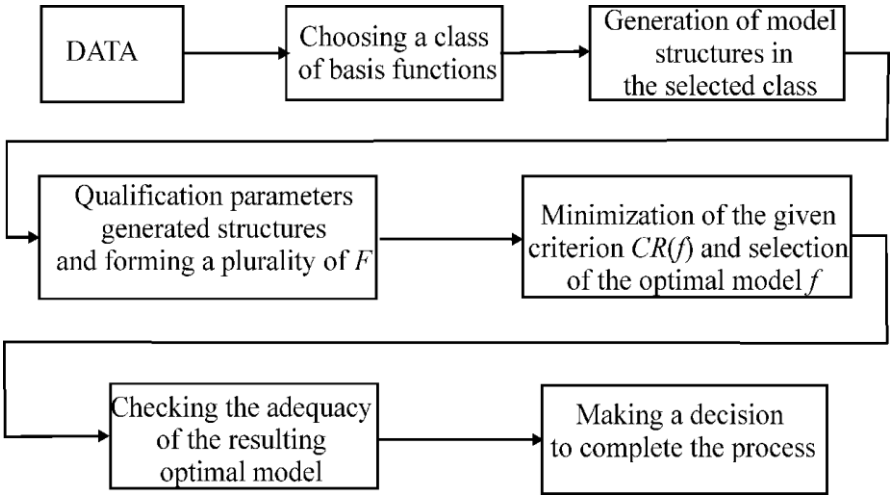


Fig. 1. General research scheme

4.1 Data

Table 1 comparatively shows the results of capillary gas-liquid chromatography with electron capture background γ-hexachlorocyclohexane (γ – HCH) and its isomers (α-HCH, β-HCH) in the whole blood of the mother and her newborn.

Table 1. The content of HCH isomers in the blood of mother and child.

Pair number	α-HCH		β-HCH		γ -HCH		∑ HCH	
«Mother-Child»	Child	Mother	Child	Mother	Child	Mother	Child	Mother
1	0,46	0,27	3,82*	3,57*	2,04	1,53	2,11	17,97
2	0,44	0,08	3,01*	0,29	2,20	0,19	0,91	7,43
3	0,81	0,08	2,61*	0,15	2,74	0,19	1,73	12,59
4	0,58	0,18	2,92*	0,91*	1,33	0,34	0,67	12,08
5	0,41	0,09	1,35*	0,58*	0,67	0,33	1,54	11,58
6	0,72	0,35	2,57*	2,72*	4,81	0,58	1,90	38,08
7	0,60	0,14	0,51*	3,82*	0,71	0,22	4,91	4,51
8	0,35	0,09	0,82*	0,48*	1,10	0,12	2,27	17,92
9	0,73	0,99	0,54*	0,69*	19,93	0,13	3,00	16,66
10	0,86	0,20	0,34*	0,34*	0,22	0,19	1,85	6,04
11	0,39	0,17	2,70*	0,18	0,95	0,19	2,66	22,49
12	0,78	0,38	1,22*	0,53*	1,19	0,35	3,83	18,59
13	0,34	0,12	1,45*	0,46*	0,81	0,35	3,27	24,72
14	0,09	0,07	0,84*	0,31*	1,88	0,13	2,60	13,86
15	0,27	0,17	1,04*	0,54*	0,71	0,15	1,81	15,00
16	0,35	0,12	0,80*	0,40*	0,51	0,14	2,21	12,39
17	0,27	0,12	1,12*	1,96*	1,95	0,26	3,05	14,37
18	0,15	0,21	0,78*	0,64*	0,29	0,20	2,99	17,59
19	0,57	0,05	0,46*	0,28	0,25	0,13	3,55	6,16
20	0,95	0,18	0,54*	0,47*	0,21	0,25	2,54	4,16
21	1,57	0,32	0,65*	0,27	0,49	0,23	1,31	3,77
22	0,15	0,08	1,22*	0,38*	2,47	0,26	1,63	13,67
23	2,23	0,20	0,91*	0,40*	0,39	0,34	1,25	7,57
24	1,16	0,33	0,56*	0,61*	0,41	0,40	0,67	5,35
25	0,27	0,16	0,54*	0,45*	0,44	0,27	2,19	20,31
26	0,57	0,22	0,33*	1,01*	0,43	0,32	10,70	10,06

Note: * - exceeding the reference value

4.2 Method

This method is based on a selection procedure that implements the process of sequential testing of models from a variety of candidates in accordance with the selected criterion. Using training with a teacher, the Group method of data handling (GMDH) allows you to find the functional dependence of the output variable on the most sig-

nificant arguments at the system input. Most GMDH algorithms use polynomials as support functions. At the same time, it is possible to use other types of nonlinear dependencies, for example, finite-difference, logistic, harmonic, etc. In accordance with the work of [11-13] method GMDH is the basis of mathematical support for direct modelling of complex systems with a small amount of experimental data. It can be expected that GMDH models will allow to obtain sufficiently accurate approximations for quantitative prediction of the content of organochlorine toxicants in the body. In general terms, the relationship between input and output variables is represented by the Volterra functional series, the discrete analog of which is the Kolmogorov-Gabor polynomial [14,15] with a general appearance:

$$y_i[n] = w_{i0} + \sum_{i=1}^{N} w_{ij} z_j[n] + \sum_{j_1=1}^{N} \sum_{j_2=j_1}^{N} w_{ij_1j_2} z_{j_1}[n] z_{j_{21}}[n] + \ldots \quad (2)$$
$$+ \sum_{j_1=1}^{N} \sum_{j_2=j_1}^{N} \ldots \sum_{j_k=j_{k-1}} w_{ij_1\ldots j_k} z_{j_1}[n] z_{j_{21}}[n] \ldots z_{jk}[n],$$

where w_{ij} is the parameters of the polynomial to be evaluated, $z_j[n]$ is the discrete values of the vector argument $z = (z_1, z_2, \ldots, z_N)^T$, N is the dimension of the vector of parameters.

According to the Stone – Weierstrass theorem, it is shown that at some degrees of arguments arbitrarily high approximation accuracy can be achieved.

Equation (3) underlies the so-called polynomial neural network [16-19]. However, for practical use, a nonlinear polynomial transformation of the argument vector into a vector of polynomials is used:

$$z \in N \to \left(\phi_1(z), \phi_2(z), \ldots, \phi_M(z)\right)^T \in M \quad (3)$$

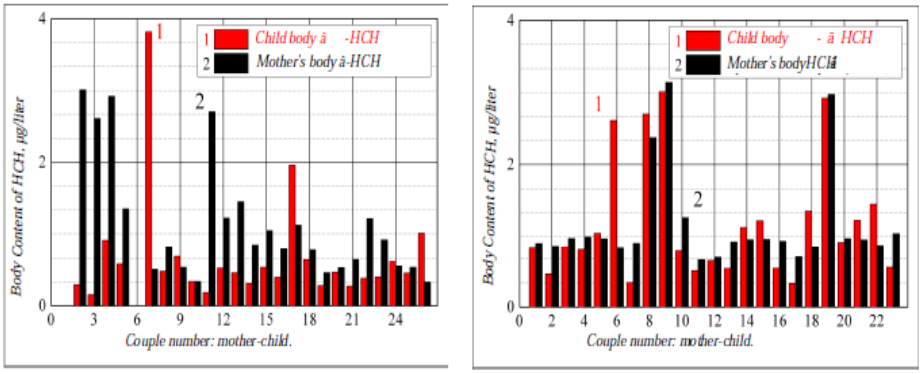
Here it is important that each of the polynomials $\phi_i(z)$ depends only on the input signal and other components of the polynomial extension and does not contain free parameters. The latter favourably distinguishes polynomial networks from popular and widely used radial-base neural networks. In addition, polynomial networks are characterized by high learning speeds, due to the fact that their output signal depends linearly on the parameters. Finally, we have:

$$y_i[n] = w_{i0} + \sum_{j=1}^{M} w_{ij} \phi_j(z[n]), i = 1, 2, \ldots, N \quad (4)$$

The consideration procedure used in GMDH is the gradual complication of partial models, ie. models with fewer components are followed by more complex models.

In practice, the described procedure of the GMDH algorithm is only a stage of a more complex scheme. Here we will consider two main schemes, called multistage combinatorial GMDH and GMDH-type neural networks.

In fig. 2 presents the results of experimental studies of the content of HCH isomers in the blood of the mother and her newborn child.



a) b)

Fig. 2. Comparison of the content of γ- and β -HCH in the blood of mother and child for individual pairs "mother-child": a) - β-HCH; b) - γ-HCH, mother and β-HCH, child. In both diagrams: columns 1 are the results of measurements in the mother's blood, columns 2 are the results in the child's blood

The results of studies of the mother's body are presented separately for γ- and β-HCH, for the child considered only β-HCH as the most dangerous, potential carcinogen: diagram a) is a comparison of β-HCH in the blood of mother and child (separate pairs "mother-child"); diagram b) is a comparison of the content of γ-HCH detected in the mother's body with the amount of β-HCH detected in the body of the child.

Despite the natural functional relationship between the data samples for mother and her child, there is due to the large number of uncontrolled parameters of biological objects very stochastic nature of the relationship between the measured values in the pair "mother-child" with sample variance for β-HCH and for γ-HCH in the mother. Comparative analysis of experimental data suggests that samples of β-HCH content for mother and her child are less correlated than samples of γ-HCH of mother and β-HCH of the child. Thus, the coefficient of cross-correlation between samples of β-HCH content for the mother and her child, while the coefficient of cross-correlation between samples of γ-HCH content for the mother and β-HCH content for her child.

In addition, the small size of the experimental samples greatly complicates the construction of prognostic models for the diagnosis of the expected content of organochlorine toxicants in the body of the newborn child based on the analysis of the mother on the basis of experimental data.

The lack of a reliable theoretical basis for the above system on the mechanisms of intrauterine transfer of organochlorine toxicants into the body of the child and increased requirements for accurate prediction necessitates the use of modern, often quite complex approaches, among which we can note the method based on artificial neural networks necessary approximating and extrapolating properties. It is clear that without taking into account the specifics of a particular task, it is impossible to choose or synthesize a neural network architecture that is best suited for this case.

5 Results and Discursion

Implementation and training of a polynomial neural network with training and test samples of 90% and 10% of the total data set, respectively, was carried out in the environment GMDH shell 3.1.4. The optimization criterion was chosen to be the minimum standard deviation between the results of model calculations and experimental data. As a model argument, we took the content of organochlorine toxicants in the mother's body. The result of the simulation was the calculation of the predicted amount of the corresponding substance in the body of the unborn child.
As a result of studying the polynomial neural network, we obtained a system of equations, which will be called the GMDH model.

Obtained as a result of the construction of the neural network, the explicit form of the GMDH model for predicting the amount of β-HCH in the child's body based on the results of the mother's analysis is represented by a system of equations:

$$\begin{cases} y(x) = -0.009 + 2.159x\phi_3(x) + 1.003\phi_3(x)\phi_2(x) \\ \quad +0.063\phi_3^2(x) + 3.136\phi_2(x) - 1.032\phi_2^2(x) \\ \phi_2(x) = 0.381 + 0.992x - 0.527x\phi_3(x) - 0.186x^2 \\ \quad +0.393\phi_3^2(x); \\ \phi_3(x) = 0.299 + 0.240\phi_6(x) + 0.353\phi_4^2(x); \\ \phi_4(x) = 1476.090 + 138\phi_6(x) + 116160\phi_6(x)\phi_5(x) - \\ \quad -113929\phi_6^2(x) - 141742\phi_5(x); \\ \phi_5(x) = 3.523 - 0.737\phi_7(x)\phi_6(x) - 8.835\phi_6(x) + \\ \quad +6.437\phi_6^2(x); \\ \phi_6(x) = 1.772 - 0.113x^2 + 1.588\phi_7(x) - 1.649\phi_7^2(x); \\ \phi_7(x) = 1.235 - 0.024x - 0.023x^2. \end{cases} \quad (5)$$

The results of forecasting according to the obtained model are presented in Fig. 3. It shows the dependence of the concentration of β-HCH in the body of the child on the concentration of β-HCH in the mother.

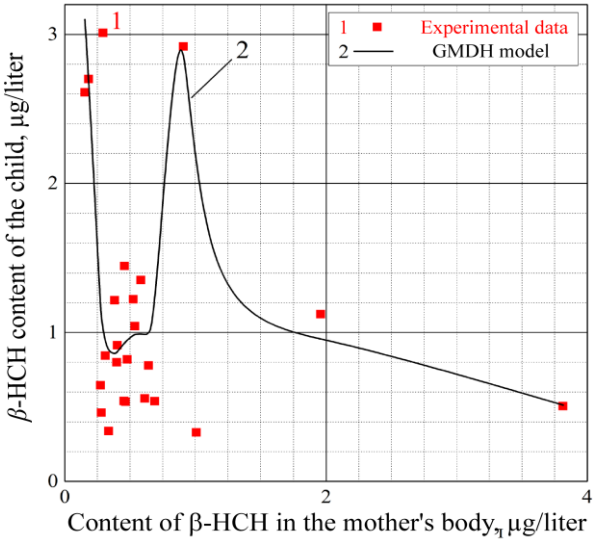


Fig. 3. Dependence of β-HCH content in the child's blood on the content of β-HCH in the mother's blood. Points 1 indicate the results of experimental measurements. Curve 2 corresponds to the calculations for the GMDH model.

Individual points 1 correspond to the experimentally established pairs of values of the concentration of β-HCH in the body of the mother and her child. The concentration of the toxicant in the mother's body was chosen as the independent variable. Solid curve 2 represents the results of the values of the concentration of β-HCH in the blood of the child calculated according to the GMDH model based on its concentration in the mother's blood.

Both experimental points and numerical approximation indicate the nonmonotonic nature of these dependencies. In the range of concentrations of the studied xenobiotic in the mother's body from 0.15 to 0.39 μg / l, there is a rapid decrease in its concentration in the body of the child from 3.10 to 0.86 μg / l. In the range of concentrations from 0.65 to 1.51 μg / l there is a sharp peak with a half-width of 0.28 μg / l, the maximum of which is the concentration of the toxicant in the mother 0.88, and reaches a concentration of 2.89 μg / l in the child. A further increase in the concentration of β-HCH in the mother from 1.51 to 3.81 μg / l is accompanied by a monotonous decrease in its concentration in the child to 0.51 μg / l.

The explicit form of the GMDH model for predicting the amount of β-HCH in the child's body based on the results of measurements of the amount of γ-HCH in the mother's body is represented by a system of equations:

$$
\begin{cases}
y(x) = 0.001 + 0.010\varphi_{12}(x)\varphi_2(x) + 0.987\varphi_2(x); \\
\varphi_2(x) = -0.497 - 0.339\varphi_9(x)\varphi_3(x) + 1.890\varphi_3(x); \\
\varphi_3(x) = -0.061 + 0.272x + 0.996\varphi_4(x); \\
\varphi_4(x) = 0.008 - 0.046\varphi_{10}{}^2(x) + 1.053\varphi_5(x); \\
\varphi_5(x) = -0.660 + 0.241\varphi_{10}(x) - 0.538\varphi_{10}(x)\varphi_6(x) + 2.030\varphi_6(x); \\
\varphi_6(x) = 0.573 + 0.370\varphi_9(x)\varphi_7(x); \\
\varphi_7(x) = 1.252 + 0.116\varphi_{11}{}^2(x) - 1.215\varphi_8(x) + 0.682\varphi_8{}^2(x); \\
\varphi_8(x) = 0.568 - 8.110\varphi_{11}(x)\varphi_9(x) + 3.893\varphi_{11}{}^2(x) + 4.264\varphi_9{}^2(x); \\
\varphi_9(x) = 0.378 + 1.843\varphi_{12}(x) - 3.541\varphi_{12}(x)\varphi_{10}(x) + 2.277\varphi_{10}{}^2(x); \\
\varphi_{10}(x) = 3.197 + 6.306\varphi_{12}(x)\varphi_{11}(x) - 2.010\varphi_{12}{}^2(x) - 7.229\varphi_{11}(x) + 0.436\varphi_{11}{}^2(x); \\
\varphi_{11}(x) = 2.063 - 33.610x + 77.317x^2; \\
\varphi_{12}(x) = 1.019.
\end{cases}
\tag{6}
$$

The results of forecasting according to the obtained model are presented in Fig. 4. It shows the dependence of the concentration of β-HCH in the child on the concentration of γ-HCH in the mother. Individual points 1 correspond to the experimentally established pairs of values of the concentration of γ-HCH in the mother and β-HCH in her child. The concentration of the toxicant in the mother's body was chosen as the independent variable. The solid curve 2 represents the results of the values of the concentration of β-HCH in the child's body calculated according to the GMDH model based on the concentration of γ-HCH in the mother's body.

Both experimental points and numerical approximation indicate the non-monotonic nature of these dependencies. In the range of γ-HCH concentrations from 0.12 to 0.85 μg / l, there is a peak concentration of β-HCH. Its half-width is 0.04 μg / l, the maximum concentration of γ-HCH is 0.15 μg / l, and reaches a value of 0.95 μg / l. Denote this peak by the letter A.

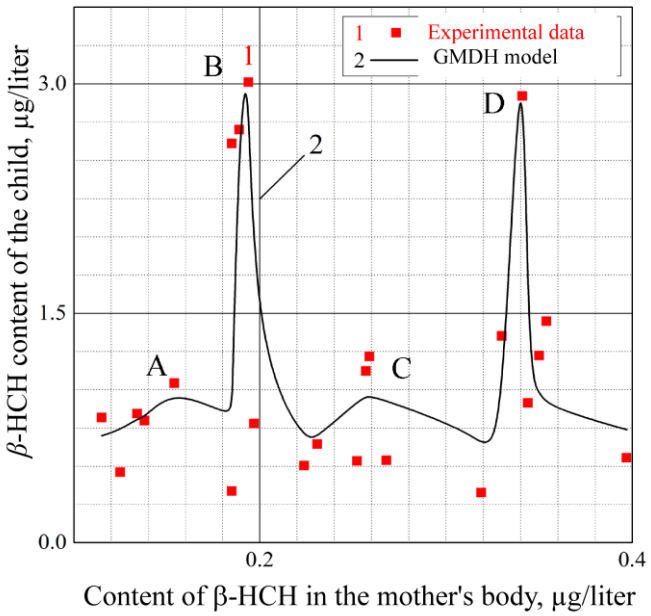


Fig. 4. Dependence of β-HCH content in the child's body on γ-HCH content in the mother's body. Points 1 indicate the results of experimental measurements. Curve 2 corresponds to the calculations for the GMDH model.

In the range of concentrations of γ-HCH from 0.18 to 0.23 μg / l, there is a sharp peak concentration of β-HCH with a half-width of 0.01 μg / l, the maximum of which is the concentration of the toxicant in the mother 0.19 μg / l and reaches the concentration of β-HCH in the child's body 2.9 mcg/liter. Denote this peak by the letter B.

In the range of γ-HCH concentrations from 0.23 to 0.67, there is a gentle peak concentration of β-HCH with a half-width of 0.05 μg / l, the maximum of which is the value of γ-HCH 0.26 μg / l and reaches the value of β-HCH in the child 0.96 μg / l with an average baseline value of 0.86 μg / l. Let it be called "peak C".

The difference between the concentration of β-HCH in the child from the concentration of γ-HCH in the mother from a similar dependence for the concentration of β - HCH in the mother is the presence of a second sharp peak ("peak D") concentration of β-HCH with a half-width of 0.01 μg / l. in the range of γ-HCH values from 0.32 to 0.36 μg / l, similar to peak B. Its maximum is at a concentration of γ-HCH 0.34 μg / l and reaches a value of 2.87 μg / l.

Further increase in the concentration in the mother from 0.36 to 0.40 μg / l is accompanied by a monotonic decrease in the concentration of β-HCH in the body of the child from 0.88 to 0.74 μg / l.

Since the difference in the concentration of flat peaks β-HCH A and C from the mean value of the baseline is 0.09 and 0.10 μg / l, which is within the statistical error of experimental data, their reliability requires additional studies to increase the size of

the statistical sample. In the framework of the presented work, they cannot be considered meaningful. That is, only peaks B and D may be of scientific interest.

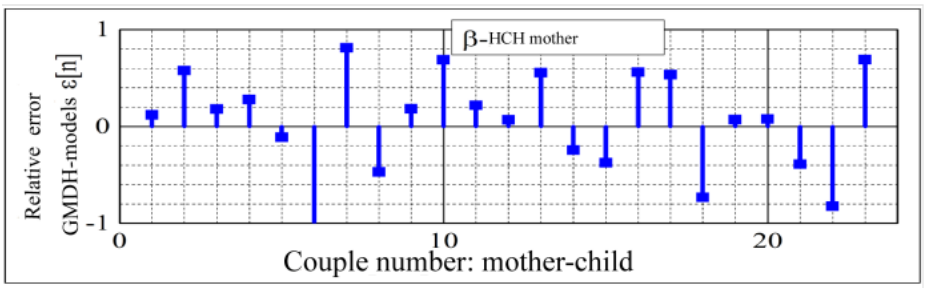
For the indicator of extrapolation and prognostic capabilities of the model chose the relative error, calculated as the difference between experimental and calculated data normalized to the variance of the sample of the amount of β-HCH in the child's body:

$$\varepsilon[n]=\frac{\xi[n]-x[n]}{\sigma_y^2}, n=1,2,...,N \qquad (7)$$

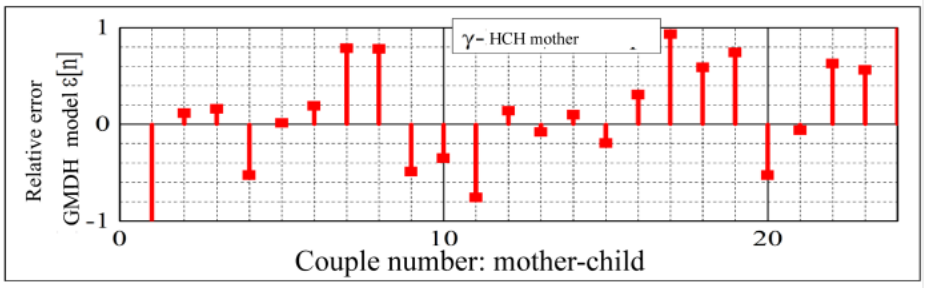
here $x[n]$ is the result of the analysis of the child's body, $\xi[n]$ is the result of calculations on the systems of equations (4, 5), representing the corresponding model, σ_y^2 is the variance of the sample analysis of the child, N is the number of studied mother-child pairs. In fig. Figure 5 shows the results of calculating the relative error of the GMDH model calculated by the formula (7).

As can be seen from the above estimates, the relative error of the constructed models on average does not exceed the statistical error of experimental studies.

An additional indicator of the quality of the model can be considered the coefficient of cross-correlation between the calculated and experimental data. Thus, for the dependence of the concentration of β-HCH in the child's body on the concentration of β-HCH in the mother's body, the mutual correlation between model and experimental data is 0.9209, and for the dependence of β-HCH concentration in the child's body on the concentration of γ-HCH in the mother's body is 0.9379.



a)



b)

Fig. 5. Relative error of GMDH model for different mother-child pairs. Graph a) corresponds to the simulation of the dependence of the content of β-HCH in the child's blood on the content of β-HCH in the mother's blood, graph b) corresponds to the dependence of the content of β-HCH in the child's blood on the content of γ-HCH in the mother's blood.

6 Conclusion

As a result of the work were:

• Numerical models based on a polynomial neural network for approximation and prediction of β-HCH concentration in the child's body based on data on the accumulation of β- and γ-HCH in the mother's body, due to the state of background contamination with persistent organochlorine compounds from among stable POPs, namely drinking water, air and food.

• The error of the models did not exceed the variance of the linear regression in the samples of experimental data. The correlation coefficients between the calculated and experimentally obtained data series were 0.9209 for the concentration of β-HCH and 0.9379 for the concentration of γ-HCH in the mother.

• Experimental studies and approximation results have shown that the dependence of the concentration of organochlorine xenobiotic in the child's body on its concentration in the mother's body is non-monotonic. In particular, it was found that there are critical concentrations of the toxicant in the mother's body at which there is an explosive transfer of stable organochlorine xenobiotics into the child's body. For β-HCH in the mother, the range of such critical concentrations is in the range of 0.60 ÷ 1.16 μg / l. For γ-HCH the intervals of critical concentrations are two and they are localized in the range of 0.18 ÷ 0.20 and 0.33 ÷ 0.35 μg / l.

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