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Interval Discrete Equation as a Model of Soil and Groundwater Contamination by Nitrogen Dioxide and Nitrogen Acid

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Task Statement

$$v_k = \vec{f}^T(v_{k-d},\dots,v_{k-1},\ \vec{u}_0,\dots,\vec{u}_{d-1},\vec{u}_k)\cdot\vec{g},\quad k=d,\dots,K\ , \tag{1}$$

where

v_k – modeled concentration of pollutants in the soil (groundwater) on discrete, specifying different depths $k = d,\dots,K$;

$\vec{u}_0,\dots,\vec{u}_k$ – vectors of input variables (meteorological conditions, humidity and soil type);

d – order of the discrete model;

$\vec{g}$ – vector of unknown model parameters;

$\vec{f}^T(\bullet)$ – vector of unknown basic functions.

$$\lambda_s = \{f_1^s(v_{k-d},\dots,v_{k-1},\vec{u}_0,\dots,\vec{u}_k)\cdot g_1^s,\ \ f_2^s(v_{k-d},\dots,v_{k-1},\vec{u}_0,\dots,\vec{u}_k)\cdot g_2^s\ ,\dots,f_m^s(v_{k-d},\dots,v_{k-1},\vec{u}_0,\dots,\vec{u}_k)\cdot g_m^s\} \tag{2}$$

$$\vec{V} = (v_{k-d},\dots,v_{k-1},\vec{u}_0,\dots,\vec{u}_k)\ , \tag{3}$$

$$\lambda_s = \{f_1^s(\vec{V})\cdot g_1^s, f_2^s(\vec{V})\cdot g_2^s,\dots,f_m^s(\vec{V})\cdot g_m^s\}\ . \tag{4}$$

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$$[z_k^-; z_k^+] \ , \ k = 0,...,K \ , \quad (5)$$

where z_k^-, z_k^+ - respectively, the lower and upper limits of the range of possible concentration values established by the results of observations in discrete $k = 0,...,K$.

Mathematical models - applicants, which will be considered in the process of structural identification, taking into account the above notation, will look like this:

$$v_k(\lambda_s) = f_1^s(\vec{V}) \cdot g_1^s + f_2^s(\vec{V}) \cdot g_2^s + ... + f_m^s(\vec{V}) \cdot g_m^s , \ k=d,...,K. \quad (6)$$

We set the conditions of consistency of the model- applicant with experimental interval data:

$$v_k(\lambda_s, \vec{V}_k) \in \left[z_k^-; z_k^+ \right], \ \forall k = 0,...,d-1, d,...,K \ , \quad (7)$$

where $v_k(\lambda_s, \vec{V}_k)$, $k = 0,...,K$ - means the true value of the initial characteristic for a fixed set of structural elements λ_s and for the fixed values of the vector $\vec{V} = (v_{k-d},...,v_{k-1}, \vec{u}_0,...,\vec{u}_k)$ represented (3) for all discrete $k = 0,...,K$.

Only the values of the parameters $g_1^s,...,g_m^s$ of the applicant model remain unknown in this case. Taking into account condition (7), we obtain the following ISNAE:

$$\begin{cases} [v_0^-; v_0^+] \subseteq [z_0^-; z_0^+], ..., [v_{d-1}^-; v_{d-1}^+] \subseteq [z_{d-1}^-; z_{d-1}^+]; \\ z_k^- \le f_1^s(\vec{V}_k) \cdot g_1^s + f_2^s(\vec{V}_k) \cdot g_2^s + ... + f_m^s(\vec{V}_k) \cdot g_m^s \le z_k^+, \\ \qquad k = d,...,K \end{cases} \quad (8)$$

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$$[\hat{v}_k(\lambda_s,[\hat{\vec{V}}_k])] = [\hat{v}_k^-(\lambda_s,[\hat{\vec{V}}_k]); \hat{v}_k^+(\lambda_s,[\hat{\vec{V}}_k])] = f_1^s([\hat{\vec{V}}_k])\cdot \hat{g}_1^s + f_2^s([\hat{\vec{V}}_k])\cdot \hat{g}_2^s + \ldots + f_m^s([\hat{\vec{V}}_k])\cdot \hat{g}_m^s \quad k = d,\ldots,K \tag{9}$$

where $[\hat{v}_k(\lambda_s,[\vec{V}_k])]$ – interval estimation of the simulated characteristic of a dynamic object on time discrete $k = d,\ldots,K$;

$\vec{\hat{g}}_l^s = (\hat{g}_{1l}^s, \hat{g}_{2l}^s, \ldots, \hat{g}_{ml}^s)^T$ – vector - column of estimates of the parameters of the model applicant with the structure λ_s, calculated on the l -th iteration;

$[\hat{\vec{V}}_k] = ([\hat{v}_{k-d}],\ldots,[\hat{v}_{k-1}],\vec{u}_0,\ldots,\vec{u}_k)$ - vector with interval components of object characteristic values calculated on the previous discrete using expression (9),

$[\hat{v}_0^-;\hat{v}_0^+] \subseteq [z_0^-;z_0^+],\ldots,[\hat{v}_{d-1}^-;\hat{v}_{d-1}^+] \subseteq [z_{d-1}^-;z_{d-1}^+]$.

Thus, the compatibility of ISNAE (8) means that the intervals of values $[\hat{v}_k(\lambda_s,[\vec{V}_k])]$ predicted characteristics in all discrete to intervals $\left[z_k^-;z_k^+\right]$, $\forall k = 0,\ldots,d-1,d,\ldots,K$, obtained experimentally, that is, for fulfilling such conditions:

$$[\hat{v}_k(\lambda_s,[\vec{V}_k])] \subset \left[z_k^-;z_k^+\right],\ \forall k = 0,\ldots,K \tag{10}$$

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The expression for the function $\delta(\lambda_s)$ that specifies the quality of the structure looks like this

$$\delta(\lambda_s) = \max_{i=1,\dots,N}\left\{\left|mid([\hat{v}_k^-(\lambda_s,[\vec{\hat{V}}_k]);\hat{v}_k^+(\lambda_s,[\vec{\hat{V}}_k])]) - mid(\left[z_k^-;z_k^+\right])\right|\right\}, \text{ if } [\hat{v}_k^-(\lambda_s,[\vec{\hat{V}}_k]);\hat{v}_k^+(\lambda_s,[\vec{\hat{V}}_k])]\cap\left[z_k^-;z_k^+\right]=\varnothing, \exists k=d,\dots,K \quad (11)$$

$$\begin{gathered}\delta(\lambda_s) = \max_{i=1,\dots,N}\{\ wid([\hat{v}_k^-(\lambda_s,[\vec{\hat{V}}_k]);\hat{v}_k^+(\lambda_s,[\vec{\hat{V}}_k])]) - \\ wid([\hat{v}_k^-(\lambda_s,[\vec{\hat{V}}_k]);\hat{v}_k^+(\lambda_s,[\vec{\hat{V}}_k])]\cap\left[z_k^-;z_k^+\right])\ \}\end{gathered},$$

$$\text{if } [\hat{v}_k^-(\lambda_s,[\vec{\hat{V}}_k]);\hat{v}_k^+(\lambda_s,[\vec{\hat{V}}_k])]\cap\left[z_k^-;z_k^+\right]\neq\varnothing, \forall k=d,\dots,K. \quad (12)$$

The problem of structural identification of interval models of dynamic objects, we formulate in the form of the following optimization problem:

$$\delta(\lambda_s)\xrightarrow{\lambda_s=\{f_1^s(\vec{V})\cdot g_{l1}^s, f_2^s(\vec{V})\cdot g_{l2}^s,\dots,f_{m_s}^s(\vec{V})\cdot g_{lm_s}^s\}}\min, \quad (13)$$

$$m_s\in[I_{\min};I_{\max}],\ f_1^s(\vec{V}), f_2^s(\vec{V}),\dots,f_{m_s}^s(\vec{V})\in F,$$

$$\hat{g}_{jl}^s\in[g_{jl}^{low};g_{jl}^{up}],\ j=1,\dots,m,\ l=1,\dots,S, \quad (14)$$

where $m_s\in[I_{\min};I_{\max}]$ – the number of structural elements of the s-th structure of the interval model; $F=\{\ f_1(\vec{V}), f_2(\vec{V}),\dots,f_m(\vec{V})\ \}$ - the set of potential structural elements of the model.

Features of Method of Structural and Parametric Identification

Initialization phase.

At this stage we set the main parameters of the method: LIMIT; S; $[I_{\min};I_{\max}]$; mcn =0 – current iteration number; MCN – the total number of iterations and the set of structural elements F, and also randomly form the initial set Λ_0 (with power S) of structures λ_s from a set of structural elements F. We use a number of operators for further formation and selection of structures.

The phase of worker bees.

In the phase of worker bees we use an operator that forms, based on each of the current structures λ_s of the mathematical model, one "new" structure λ'_s, which is close to the current in a random way and replacement of some elements of the current structure λ_s, and the replacement itself is also carried out by randomly selected elements from the set, to those selected from the set F. Next, in this phase, we perform pairwise selection to select the best structure from two λ_s, λ'_s: the current and the generated.

Phase of researchers bees.

In this phase, we determine the number of structures that will be generated based on each current structure. To do this, we use the probabilistic approach. The better the structure, the more modifications we will form on its basis. To modify the structures, we use an operator that replaces the elements of each (or some structures) randomly. This replacement is also performed by randomly selected elements from the set. Exit from the local minima of the objective function of problem (13), (14) is carried out on the phase of scout bees

Phase of scout bees.

This is the phase of bees that choose new sources of nectar at random, ie it means that in this phase it is necessary to randomly form new structures, in the manner described in the initialization phase. To do this, for each for each current structure, we introduce a counter, which in the context of the behavioral model of the bee colony simulates the process of reducing the amount of nectar in accordance with the procedure for identifying depleted sources of nectar.

Mathematical Models of Nitrogen dioxide diffusion in Soil and Waterbody

$$2NO_2 + H_2O \rightarrow HNO_3 + HNO_2$$

$$3HNO_2 \rightarrow HNO_3 + 2NO + H_2O$$

$$6NO_2 + 3H_2O \rightarrow 4HNO_3 + 2NO + H_2O$$

$$3NO_2 + H_2O \rightarrow 2HNO_3 + NO$$

To build this model, we use the results of the representation of the concentrations of nitrogen dioxide or salts of nitric acid. Table 1 shows the results of the evaluation of these contaminants at a depth of up to 14 centimeters with a discrete of 2 cm, k = 0… 7.

TABLE I. NITROGEN DIOXIDE AND ACID MEASUREMENT RESULTS.

Number of discretes	**Dipth, m**	**1st point,** Concentration of Nitrogen dioxide, $10^{-6}\frac{g}{m^3}$,	**2nd point** Concentration of Nitrogen dioxide, $10^{-6}\frac{g}{m^3}$,	**3th point** Concentration of Nitrogen dioxide, $10^{-6}\frac{g}{m^3}$,
k	h	z_k		
0	0	14	14,8	13,1
1	0,02	13,8	14,1	12,8
2	0,04	10	10,1	8,9
3	0,06	5	5,1	3,8
4	0,08	1	1,2	0,4
5	0,1	0	0	0
6	0,12	0	0	0
7	0,14	0	0	0

Mathematical Models of Nitrogen dioxide diffusion in Soil and Waterbody

To build the model, the initial conditions were given in the following discrete: k = 0, 1 and with an interval extension of ± 0.5%. At the same time, during the simulation the experimental data were given with an interval extension of ± 10%.

TABLE II. SET OF THE GENERATED POTENTIAL STRUCTURAL ELEMENTS OF THE MODEL

№	Structural element	№	Structural element
1	v_{k-1}	6	v_{k-3}^2
2	v_{k-2}	7	$v_{k-1} \cdot v_{k-2}$
3	v_{k-3}	8	$v_{k-1} \cdot v_{k-3}$
4	v_{k-1}^2	9	$v_{k-2} \cdot v_{k-3}$
5	v_{k-2}^2	10	$v_{k-1} \cdot v_{k-2} \cdot v_{k-3}$

$$[\hat{v}_k^-, \hat{v}_k^+] = -0.01675 \cdot [\hat{v}_{k-2}^-, \hat{v}_{k-2}^+] + \\ +0.05269 \cdot [\hat{v}_{k-1}^-, \hat{v}_{k-1}^+] \cdot [\hat{v}_{k-1}^-, \hat{v}_{k-1}^+]. \qquad (15)$$

Mathematical Models of Nitrogen dioxide diffusion in Soil and Waterbody

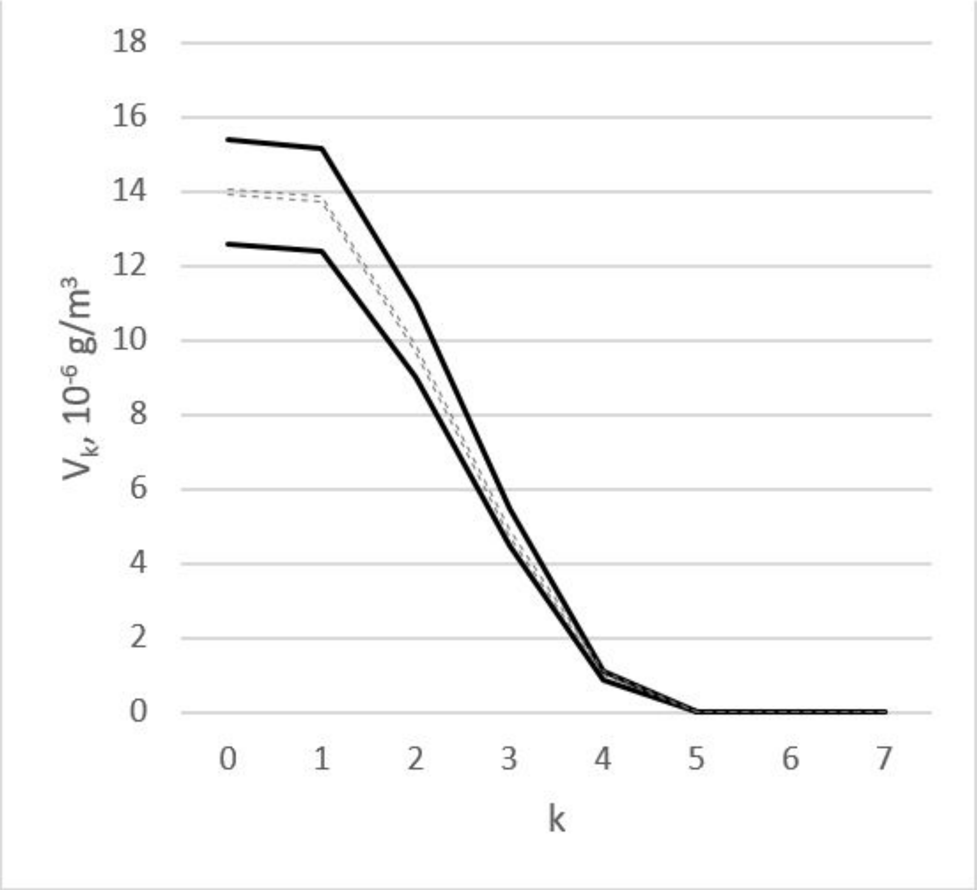

Fig.1. Predicted values of nitrogen dioxide concentrations for the first measurement point from table 1.

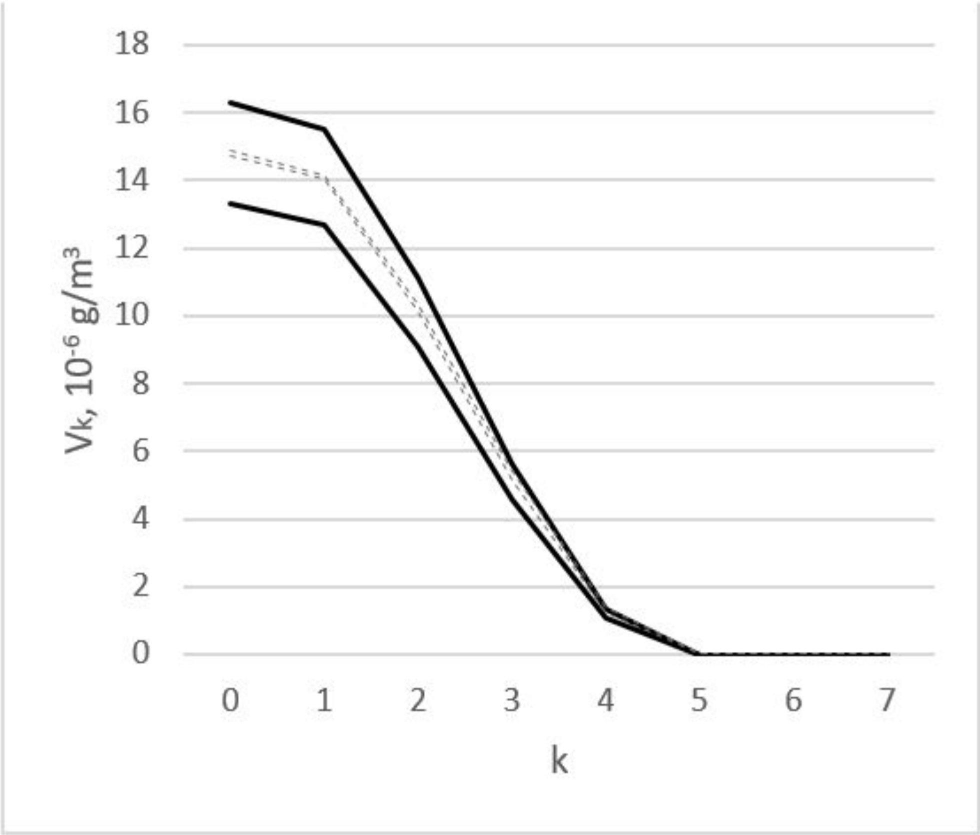

Fig.2. Predicted values of nitrogen dioxide concentrations for the second measurement point from table 1.

Mathematical Models of Nitrogen dioxide diffusion in Soil and Waterbody

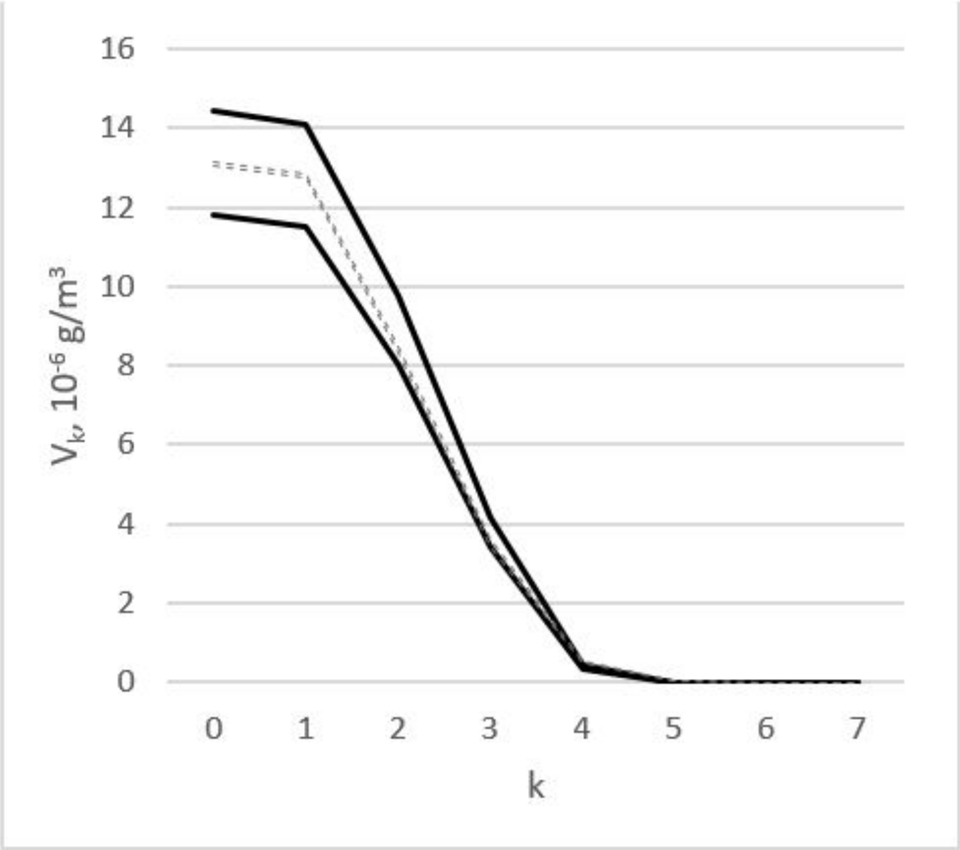

Fig.3. Predicted values of nitrogen dioxide concentrations for the third measurement point from table 1.

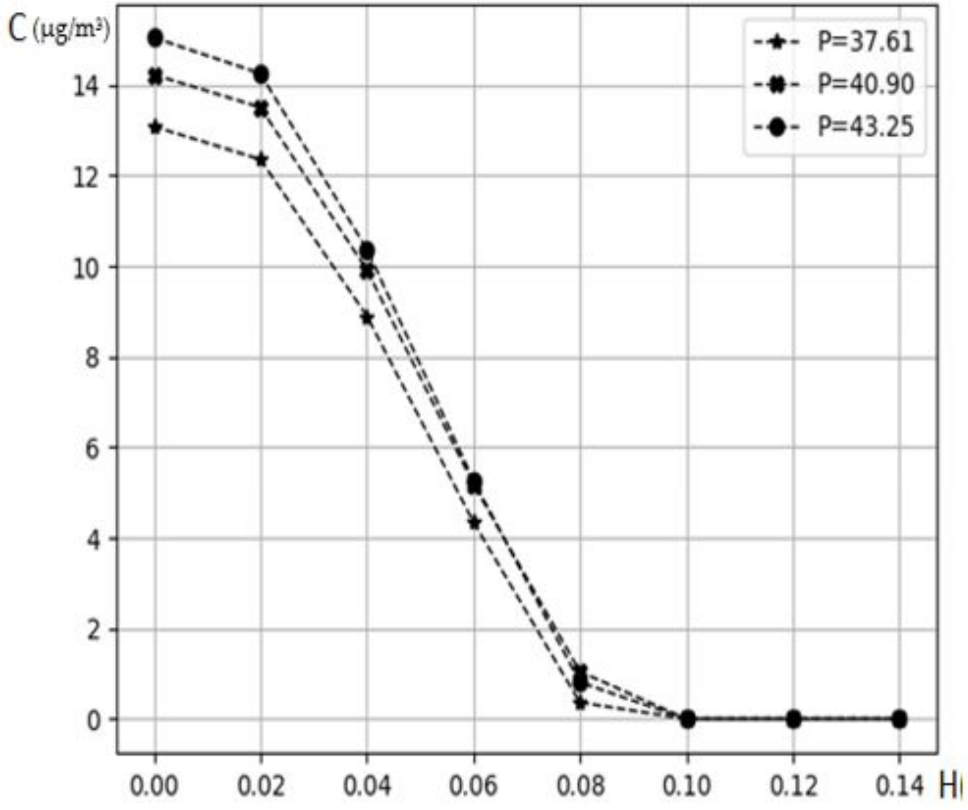

Fig. 4. The results of modeling the diffusion of nitrogen dioxide and nitric acid.

Conclusions

The results of the construction of Interval Discrete Equation as a Model of Soil and Groundwater Contamination are given.

It is proposed to solve the problem of modeling the processes of soil contamination with nitrogen dioxide and nitric acid salts with the help of a difference operator.

To identify it, a method of identification of this model is proposed, which is based on the behavioral models of the bee colony.

The simulation results show that the obtained interval discrete model adequately describes the processes of diffusion of nitrogen dioxide in the soil with a given accuracy.

Thank you for attention!