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MODELING OF DISSOLUTION, ION EXCHANGE AND ADSORPTION IN SOILS

The presented article is devoted to constructing regression models of the processes of dissolution, ion exchange and adsorption to create simulation systems in order to optimize the quality of soils.

Keywords: sanitary and epidemiological situation, prediction, operational management, computer simulation experiments, the regression models.

Problem statement.

The problem of "soil - a man" is complicated by urbanization, the increasing use of land, its resources for industry and house building, increasing demand for food. By the man's will the nature of the soil, soil factors - topography, climate – are changing [1]. Under the influence of industrial and agricultural pollution the properties of soil and soil-forming process, potential fertility changes, reduces technological and nutritional value of agricultural products etc. The author of the fundamental work in ecology J. Odum points out that "pollution - are the natural resources that were replaced," because they are alien to natural ecosystems and accumulate in them breaking the cycle of matter and energy, reducing their performance impact on human health [2]. All this also influences on the sanitary-epidemiological status of the region.

Analysis and prediction of sanitary and epidemiological situation, research for management solutions and scenarios for emergency response are impossible without the use of mathematical models [3].

Analysis of recent research and publications.

Among the works on optimization ecoareas and those dealing with the processes related to the prediction and optimization of the quality of air, soil and water pollution, stands the fundamental three-volumed monograph by Goryeva L.M., Doroguntsov S.I. and Hvesyka M.A. "Optimization of ecoareas" [4]. Created by authors adequate mathematical models related processes let to simulate the most favorable conditions for the functioning of natural and industrial environments. Computerization of simulation systems allows to find efficiently the best options for the functioning of these environments and prevent the occurrence of extra situations. But in order that the simulation systems could be part of SPPR, it is necessary to simplify the numerical solution of differential equations describing processes in ecoarea, by building sufficiently accurate approximation equations. This greatly simplifies the use of simulation models and makes quite convenient for practical implementation, as elements of SPPR.

The objective of the article.

Development of methods for assessing the ion exchange process between rock and water solution, building regression models of the processes of dissolution and sorption simpler and more convenient for practical use, and the creation of simulation systems to optimize the quality of soils.

Presentation of main material.

The mass transfer processes occurring in equilibrium hydrochemical systems include processes of dissolution, ion exchange, adsorption (desorption), negative and positive adsorption, molecular, thermal and barodifusion, osmosis.

Under dissolving we understand the transition of molecules and ions of solid, liquid or gaseous substances in the adjacent phase as a result of thermal motion of particles of matter, soluble and solvent. A substance that is dissolved in a solvent, can chemically interact with it on the release or absorption of energy. The process of dissolution is accompanied by diffusion, which resulted in molecules that move from one phase to another, evenly distributed throughout the volume of the solvent. The degree of solubility of a substance in a given solvent is the concentration of its saturated solution. Dissolution greatly affects the ion-salt composition of groundwater if that soil, rock zone aeration and water-containing rocks contain

significant amounts of soluble salts or even salt belt and layers. Solubility of salts in natural waters strongly depends on temperature, pressure, presence of other salts in solution.

Ion exchange, adsorption or exchange - this process of absorption of the surface layer of the adsorbent ions from electrolyte solutions, accompanied dissolves equivalent amount of ions absorbed by adsorbent before. In accordance with the sign of ions exchanged, adsorbents (resin) are divided into cations and anions.

An important role is played by ionic processes in the following cases:

- in conditions of unsustainable lithium salt regime where a change in the concentrations of individual components in solution gives the ion-exchange equilibrium between liquid and colloidal and solid phases;
- when receiving irrigation water salinity in small breed aeration zone and groundwater;
- when receiving treatment increased mineralization in unsalted rocks;
- when mixing groundwater with different chemical composition;
- when entering water in water-containing rocks or soils that differ in composition from those where the water was formed;
- when you change the acid-base conditions in the water;
- when entering the soil and rock water cationic composition which differs from the cation exchange complex composition of the solid phase;
- in case of large amplitude oscillations of dispersion of water-containing area.

The mathematical model of the algorithm for estimating the ion exchange process in soils.

To evaluate the ion exchange process between rock and water solution in natural conditions, the following algorithm should be used:

$$\begin{gathered} C_p \geq C^{**} \geq 0; \\ \left(N_0 - N_p\right)\delta 10^{-3}\left\{\exp\left[\frac{\tau}{\tau_k}\ln\frac{\left(N_0 - N_p\right)\delta 10^{-3} - \left(C_0 - C_k\right)}{\left(N_0 - N_p\right)\delta 10^{-3}}\right] - 1\right\} + C_0 = C^{**}; \\ T_0 \leq T \leq T_1,\ C_p^* \geq C^* \geq 0; \\ C^{**}\exp\left(\frac{T_0 - T}{T_0 - T_1}\ln\frac{C_p^*}{C_p}\right) = C^*; \end{gathered} \tag{1}$$

$$\begin{gathered} W_1 > W_0,\ W_1 \leq W \leq W_n,\ C_p^* \geq C \geq 0; \\ C^*\exp\left(\frac{W_0 - W}{W_0 - W_1}\ln\frac{C_1}{C_0}\right) = C; \end{gathered} \tag{2}$$

where C_p, N_p - ion concentration in solution and in the exchange complex in terms of ion-exchange equilibrium; N_0, C_0 - according to the content of the ion exchange complex in solution at $\tau = 0$; $C_к$ - ion concentration in solution at $\tau = \tau_{до}$; C_p^*, C_p^{**} - equilibrium concentration of ions in solution at $T = T_1$ i $P = P_1$; T_0, P_0 - the temperature and pressure which identifies C_p, N_0, C_0 i $C_к$; T_1, P_1 - temperature and pressure, which are determined by the value of * i Cp**; $\tau_{до}$ - the time after which after the onset of ion exchange is determined by the value $C_к$; δ - density of the exchange complex; W_1, $W_п$, W_0 - hygroscopic moisture soils, humidity, level of full moisture capacity, moisture content at which the determined value of C_0; C_1 - ion concentration in a solution with a moisture content soils equal to W_1, δ - density of soils.

A mathematical model of the algorithm for estimating dissolution processes in experimental conditions.

The algorithm processes of sorption (desorption) are based on the solution of linear sorption isotherms equation in partial derivatives:

$$dC/d\tau = \beta\left(N - N_p\right), \tag{3}$$

where C - concentration of ions in solution; N_p, N - equilibrium and the observed sorption capacity of rocks; β^*- coefficient rate of sorption (desorption). In natural and experimental conditions algorithms have look almost similar to the description given for the ion exchange process:

$$C_p \geq C^{**} \geq 0;$$

$$\left(N_0 - N_p\right)\delta 10^{-3}\left\{\exp\left[\frac{\tau}{\tau_k}\ln\frac{\left(N_0 - N_p\right)\delta 10^{-3} - \left(C_0 - C_k\right)}{\left(N_0 - N_p\right)\delta 10^{-3}}\right] - 1\right\} + C_0 = C^{**};$$

$$T_0 \leq T \leq T_1\,,\; C_p^* \geq C^* \geq 0; \tag{4}$$

$$C^{**}\exp\left(\frac{T_0 - T}{T_0 - T_1}\ln\frac{C_p^*}{C_p}\right) = C^*;$$

$$P_0 \leq P \leq P_1\,,\; C_p^{**} \geq C \geq 0;$$

$$C^*\exp\left(\frac{P_0 - P}{P_0 - P_1}\ln\frac{C_p^{**}}{C_p}\right) = C; \tag{5}$$

where C_p, $\mathbf{N_p}$ - ion concentration in solution and in the exchange complex in terms of ion-exchange equilibrium; $\mathbf{N_0}$, $\mathbf{C_0}$- according to the content of the ion exchange complex in solution at $\boldsymbol{\tau = 0}$; $\mathbf{C_к}$ - ion concentration in solution at $\boldsymbol{\tau = \tau_{до}}$; $\mathbf{C_p^*}$, $\mathbf{C_p^{**}}$- equilibrium concentration of ions in solution at $\mathbf{T = T_1}$ **and** $\mathbf{P = P_1}$; $\mathbf{T_0}$, $\mathbf{P_0}$ - the temperature and pressure at which identifies the value of $\mathbf{C_p}$, $\mathbf{N_0}$, $\mathbf{C_0}$ **and** $\mathbf{C_к}$; $\mathbf{T_1}$, $\mathbf{P_1}$- temperature and pressure, which are determined by the value of C_p^* i Cp^{**}; $\tau_{до}$ - the time after which after the onset of ion exchange is determined by the value of $C_к$; δ - density of the exchange complex.

Computational simulation experiments.

Based on the results of computational experiments the approximating nonlinear regression models were built [5,6]. In the rather widely values the following process parameters varied: humidity (Wn - 15 to 30) and temperature (Tn - from 293 to 302°K), the duration of the process (TMn - from 4 to 34 hours.).
Linear regression equation has the form:

$$C = 0{,}028305 - 0{,}00063W \tag{6}$$

Quadratic regression equation has the form:

$$C = 0{,}036177 - 0{,}001319\,W - 0{,}0000147\,W^2 \tag{7}$$

Figures 1 and 2 show the simulation results depending on the concentration of chloride ions (C - kmol / m^3), which is formed by the process of dissolution of soil moisture.

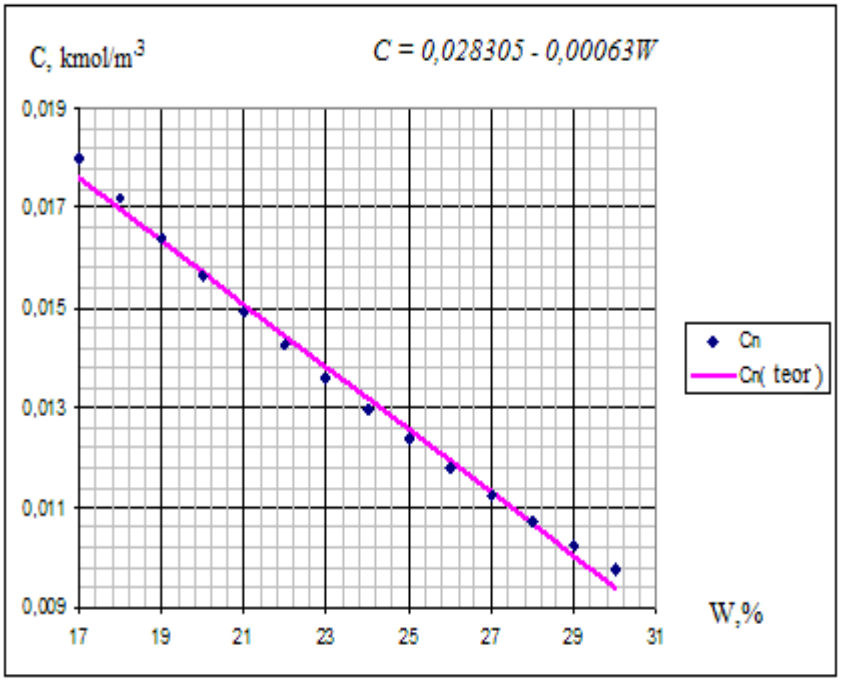


Fig. 1 - Dependence of the concentration of chloride ions from soil moisture (linear approximation)
R2 = 0,993; σ = 0,00023

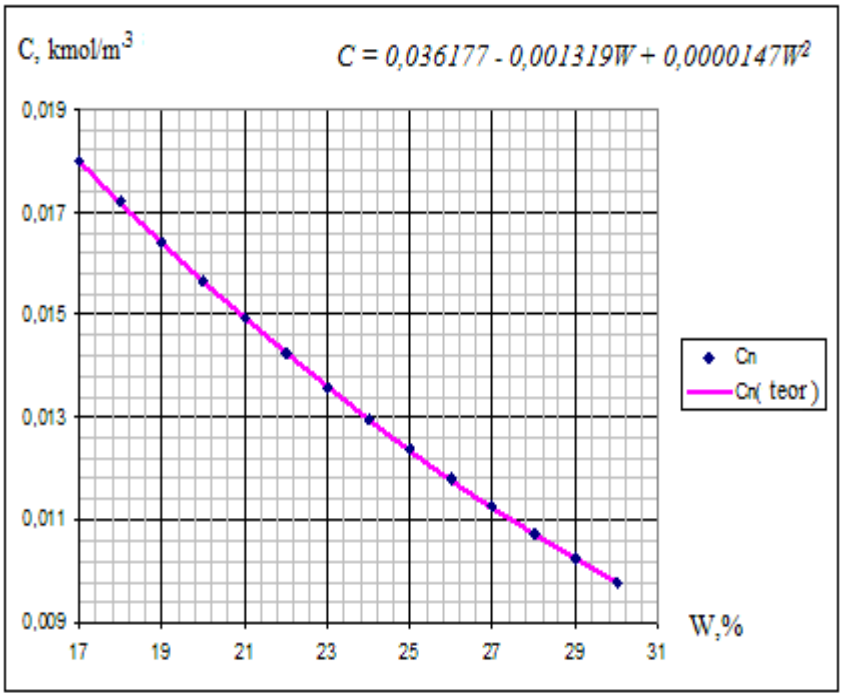


Fig. 2 - Dependence of the concentration of chloride ions from soil moisture (quadratic approximation)
R2 = 0,99998; σ = 0,0000116

The dependence of the dissolution time of humidity is presented in Figures 3 and 4.

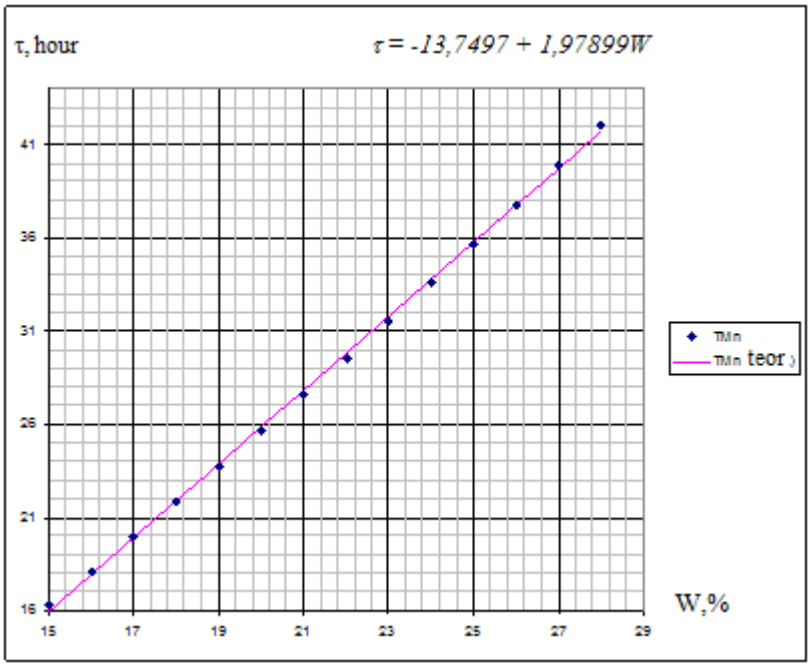


Fig. 3 - Dependence of dissolution time from moisture C=0,0141, (linear approximation)
R2 = 0,9993; σ = 0,2272

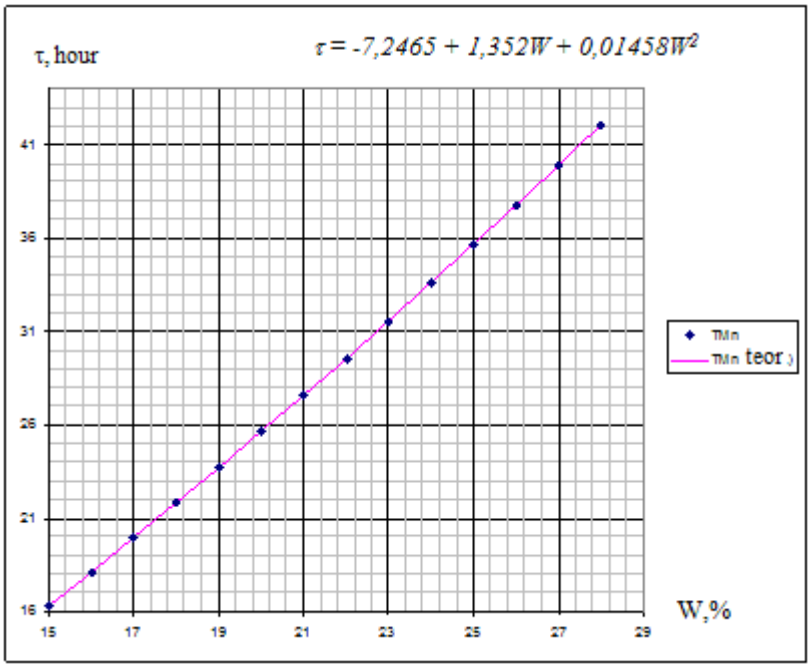


Fig. 4 - Dependence of dissolution time from the moisture C=0,0141 (quadratic approximation)
R2 = 0,99999; σ = 0,0062

Data Flow Diagrams (DFD) is the primary means of modeling the functional requirements of the system are divided into functional components (processes) and represented as a network related data streams. The main purpose of such funds - to show how each process converts its input to output, and identify relationships between these processes.

The initial context diagram is shown in Figure 5.

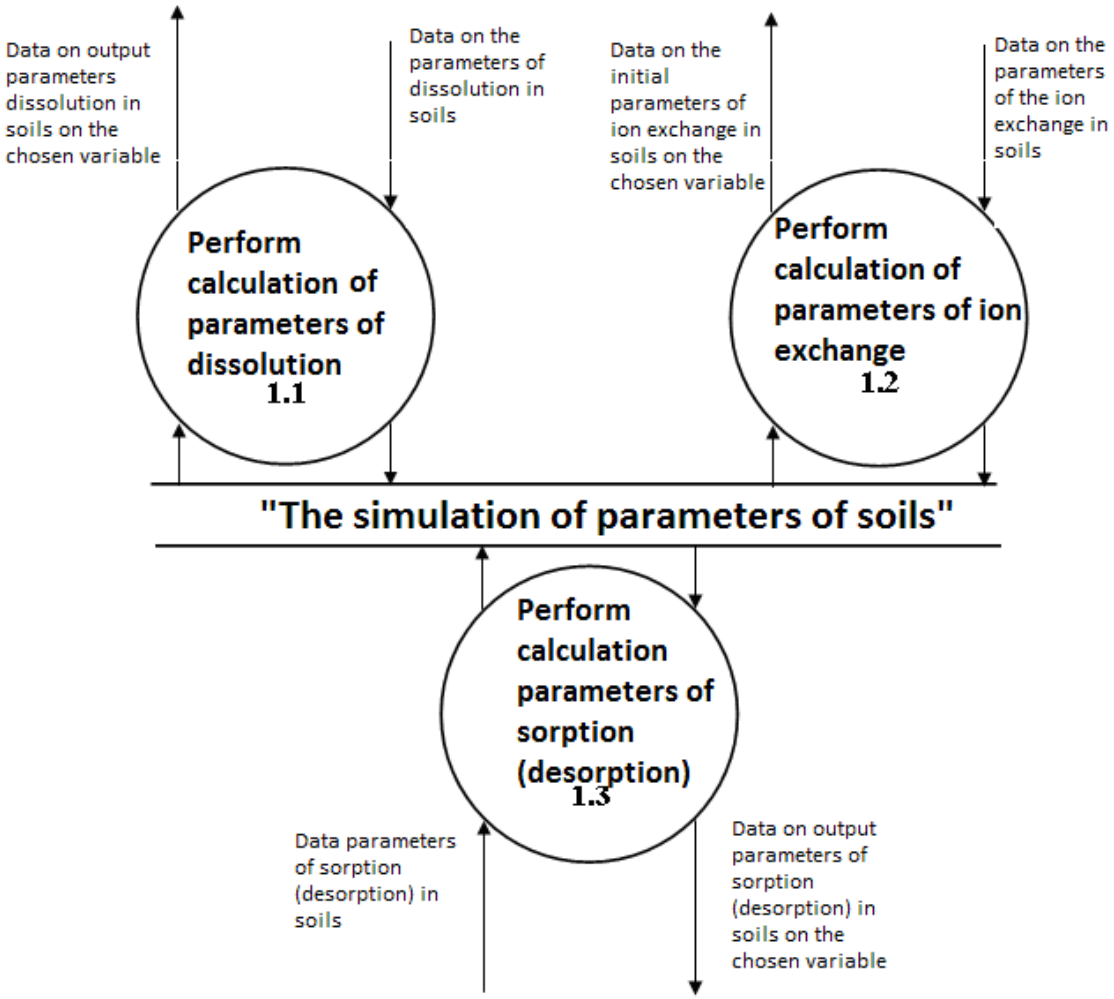


Fig. 5 - Context diagram of the second level

Events list shows which streams are at this level, every event from the list should form a stream (event forms the input stream, the reaction - the output stream). The algorithm calculates the parameters of dissolution, ion exchange and sorption (desorption) is implemented as a separate software module using the concept of object-oriented programming. Module consists of object realization that calculates the parameters of above processes. To the main program module is connected with the operator, then a variable is created that has the type of object used (called an instance of an object). The object has a constructor to initialize the object, typically setting the input field values object rule calculations and the results and destructor.

The software of formulated and algorythmized mathematical models performed only in complex, user-friendly, and performs the following functions:

- simulation of dissolution processes, ion exchange, adsorption (desorption) in soils;
- determination of the concentration;
- definition of time;
- determination of temperature;
- determination of moisture.

The algorithm calculates the parameters of dissolution, ion exchange and adsorption (desorption), implemented as a separate software module. The software of defined and algorithmised mathematical models is the only complex that is convenient for the user. Screen forms are implemented as a standard window interface of Windows, using components of the development environment Borland Delphi7.

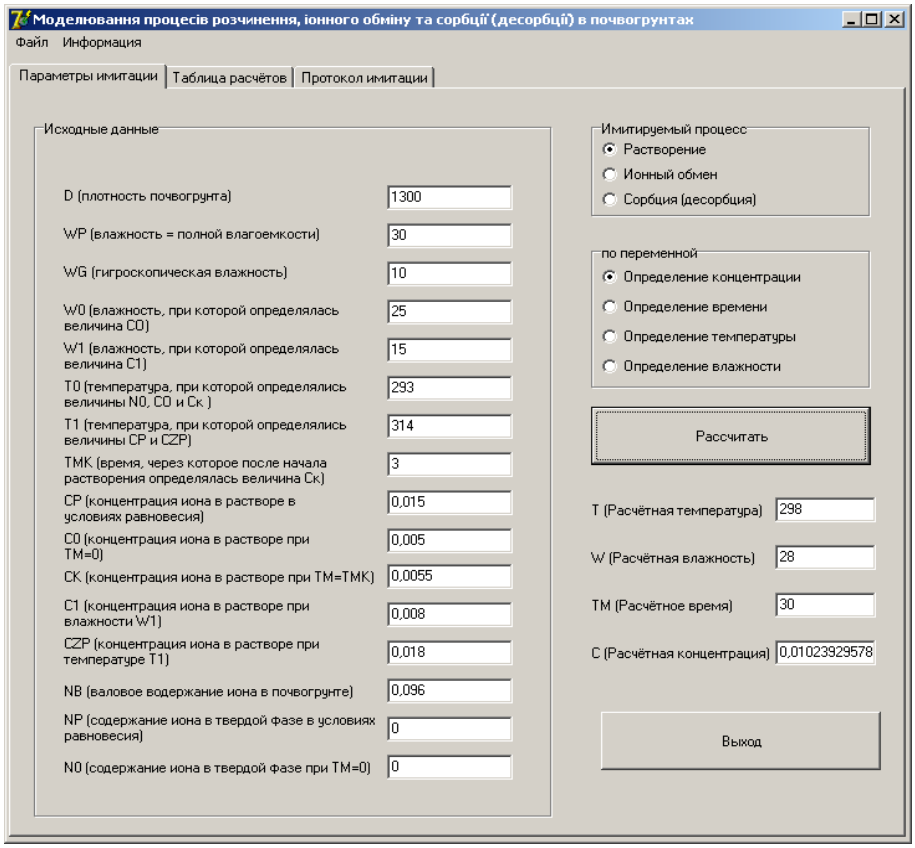
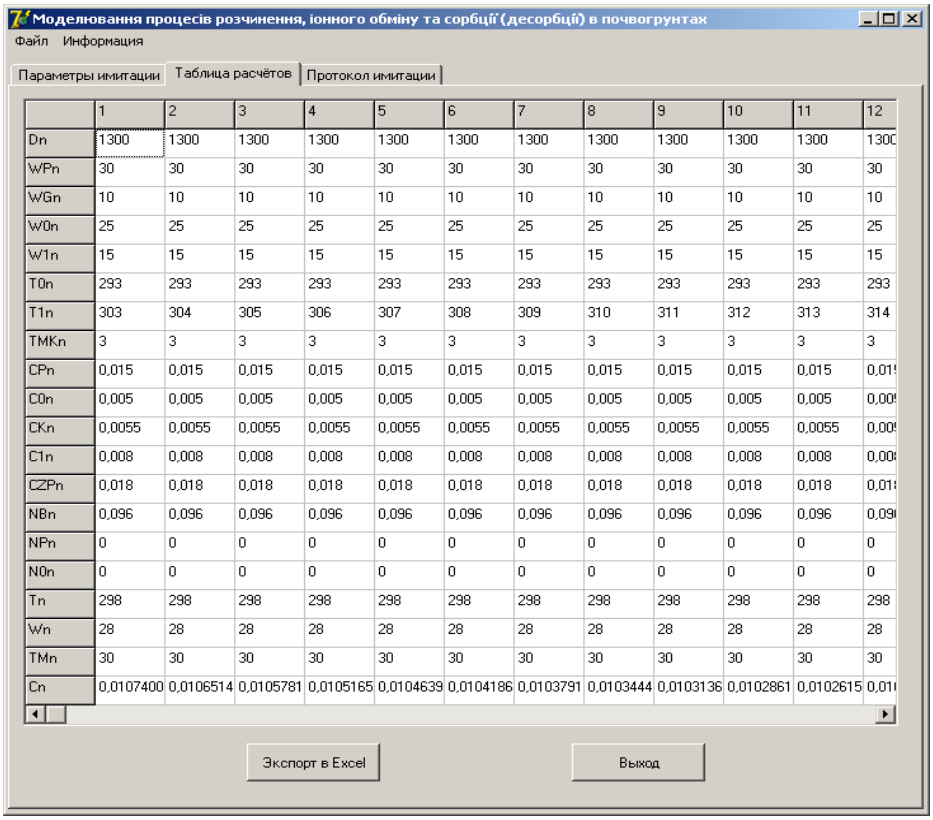


Fig. 6 - Screenshot of the program and an example of calculation of process of dissolution of the variable C (determination of concentration) in simulating mode.



	1	2	3	4	5	6	7	8	9	10	11	12
Dn	1300	1300	1300	1300	1300	1300	1300	1300	1300	1300	1300	1300
WPn	30	30	30	30	30	30	30	30	30	30	30	30
WGn	10	10	10	10	10	10	10	10	10	10	10	10
W0n	25	25	25	25	25	25	25	25	25	25	25	25
W1n	15	15	15	15	15	15	15	15	15	15	15	15
T0n	293	293	293	293	293	293	293	293	293	293	293	293
T1n	303	304	305	306	307	308	309	310	311	312	313	314
TMKn	3	3	3	3	3	3	3	3	3	3	3	3
CPn	0,015	0,015	0,015	0,015	0,015	0,015	0,015	0,015	0,015	0,015	0,015	0,01
C0n	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,00
CKn	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,00
C1n	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,00
CZPn	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,01
NBn	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,09
NPn	0	0	0	0	0	0	0	0	0	0	0	0
N0n	0	0	0	0	0	0	0	0	0	0	0	0
Tn	298	298	298	298	298	298	298	298	298	298	298	298
Wn	28	28	28	28	28	28	28	28	28	28	28	28
TMn	30	30	30	30	30	30	30	30	30	30	30	30
Cn	0,0107400	0,0106514	0,0105781	0,0105165	0,0104639	0,0104186	0,0103791	0,0103444	0,0103136	0,0102861	0,0102615	0,01

Fig. 7 - Screenshot of the program - Table accumulation of a series of calculations to be exported to an external application (Microsoft Excel).

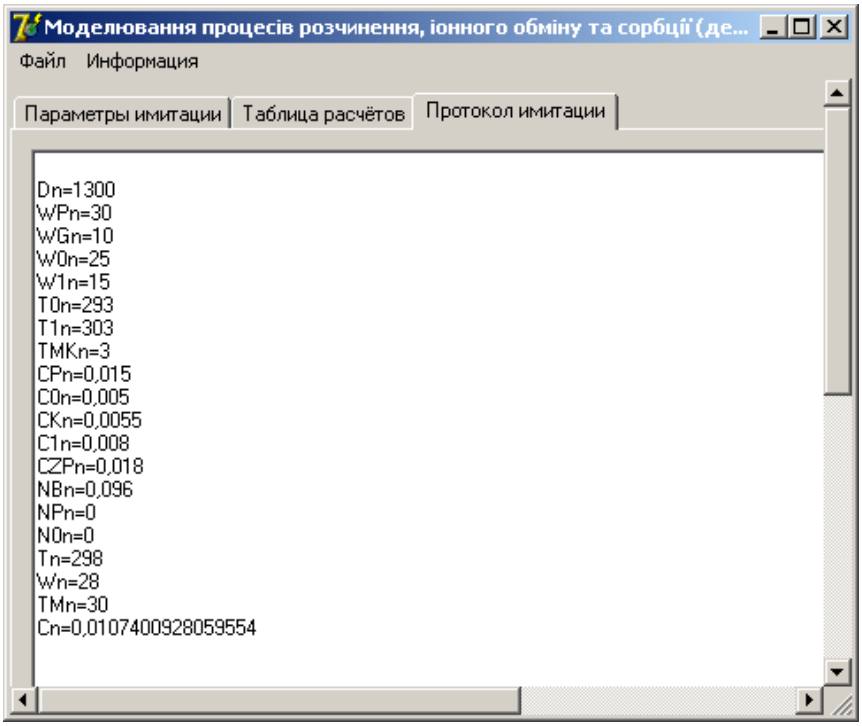


Fig.8 - Screenshot of the program (protocol simulation).

Conclusion.

The series of simulation computational experiments is conducted, on which fairly accurate regression models were built, easier and more convenient for practical use.

Implemented in the work algorithms can be a part of SPPR analysis of sanitary and epidemic emergencies and can be used to create simulation systems in order to optimize the quality of soils.

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