

## MODELING OF DISSOLUTION, ION EXCHANGE AND ADSORPTION IN SOILS

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**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.**

**Key words: 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:

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

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

$$T_0 \leq T \leq T_1, C_p \geq C^* \geq 0;$$

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

$$W_1 > W_0, W_1 \leq W \leq W_n, C_p^* \geq C \geq 0;$$

$$C^* \exp \left( \frac{W_0 - W}{W_0 - W_1} \ln \frac{C_1}{C_0} \right) = C;$$

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  $\tau = 0$ ;  $C_k$  – ion concentration in solution at  $\tau = \tau_{\text{до}}$ ;  $C_p^*, C_p^{**}$  – 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  $C_k$ ;  $T_1, P_1$  – temperature and pressure, which are determined by the value of  $C_p^*$  i  $C_p^{**}$ ;  $\tau_{\text{до}}$  – the time after which after the onset of ion exchange is determined by the value  $C_k$ ;  $\delta$  – density of the exchange complex;  $W_1, W_n, W_0$  – 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  $W_1$ ,  $\delta$  – 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:

$$dC/dt = b(N - N_p), \quad (3)$$

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

$$C_p \geq C^{**} \geq 0; \\ (N_0 - N_p)d10^{-3} \left\{ \exp \left[ \frac{t}{t_k} \ln \frac{(N_0 - N_p)d10^{-3} - (C_0 - C_k)}{(N_0 - N_p)d10^{-3}} \right] - 1 \right\} + C_0 = C^{**}; \quad (4)$$

$$T_0 \leq T \leq T_1, C_p^* \geq C^* \geq 0;$$

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

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

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

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  $t = 0$ ;  $C_k$  – ion concentration in solution at  $t = t_{до}$ ;  $C_p^*$ ,  $C_p^{**}$  – equilibrium concentration of ions in solution at  $T = T_1$  and  $P = P_1$ ;  $T_0$ ,  $P_0$  – the temperature and pressure at which identifies the value of  $C_p$ ,  $N_0$ ,  $C_0$  and  $C_k$ ;  $T_1$ ,  $P_1$  – temperature and pressure, which are determined by the value of  $C_p^*$  i  $C_p^{**}$ ;  $t_{до}$  – the time after which after the onset of ion exchange is determined by the value of  $C_k$ ;  $\delta$  – 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 ( $W_n$  – 15 to 30) and temperature ( $T_n$  – from 293 to 302°K), the duration of the process ( $TM_n$  – from 4 to 34 hours.).

Linear regression equation has the form:

$$C = 0,028305 - 0,00063W \quad (6)$$

Quadratic regression equation has the form:

$$C = 0,036177 - 0,001319W - 0,0000147W^2 \quad (7)$$

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

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

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. 1. Dependence of the concentration of chloride ions from soil moisture (linear approximation)  $R^2 = 0,993$ ;  $\sigma = 0,00023$

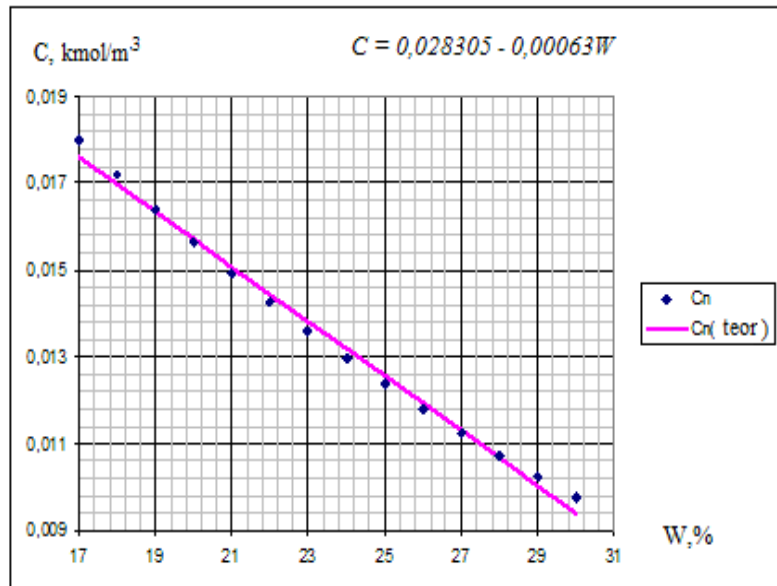


Fig. 2. Dependence of the concentration of chloride ions from soil moisture (quadratic approximation)  $R^2 = 0,99998$ ;  $\sigma = 0,0000116$

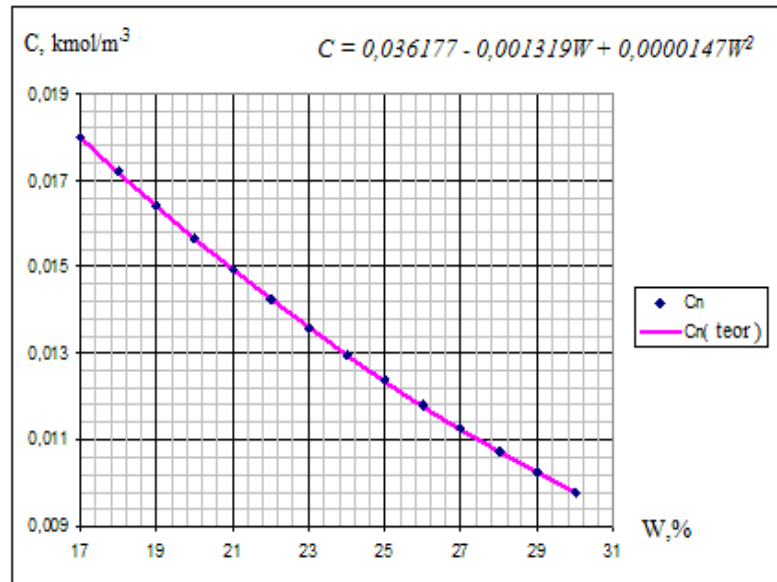
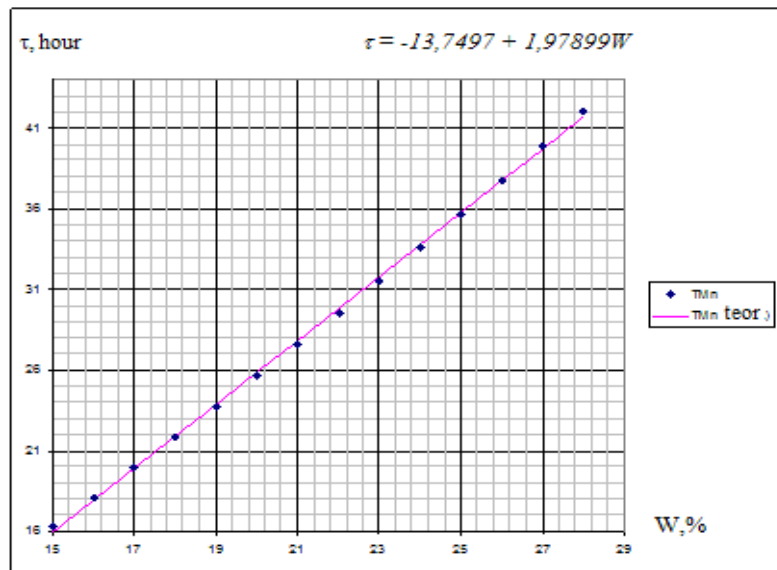


Fig. 3. Dependence of dissolution time from moisture  $C=0,0141$ , (linear approximation)  $R^2 = 0,9993$ ;  $\sigma = 0,2272$



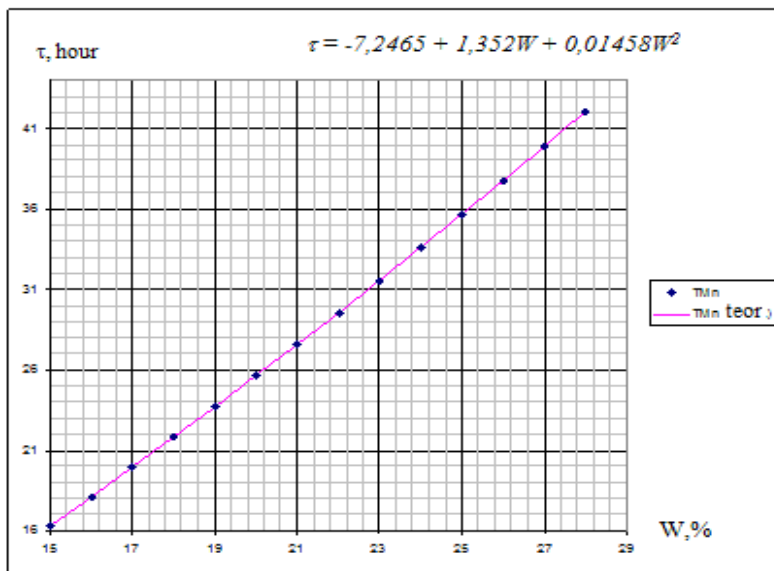


Fig. 4. Dependence of dissolution time from the moisture  $C=0,0141$  (quadratic approximation)  $R^2 = 0,99999$ ;  $\sigma = 0,0062$

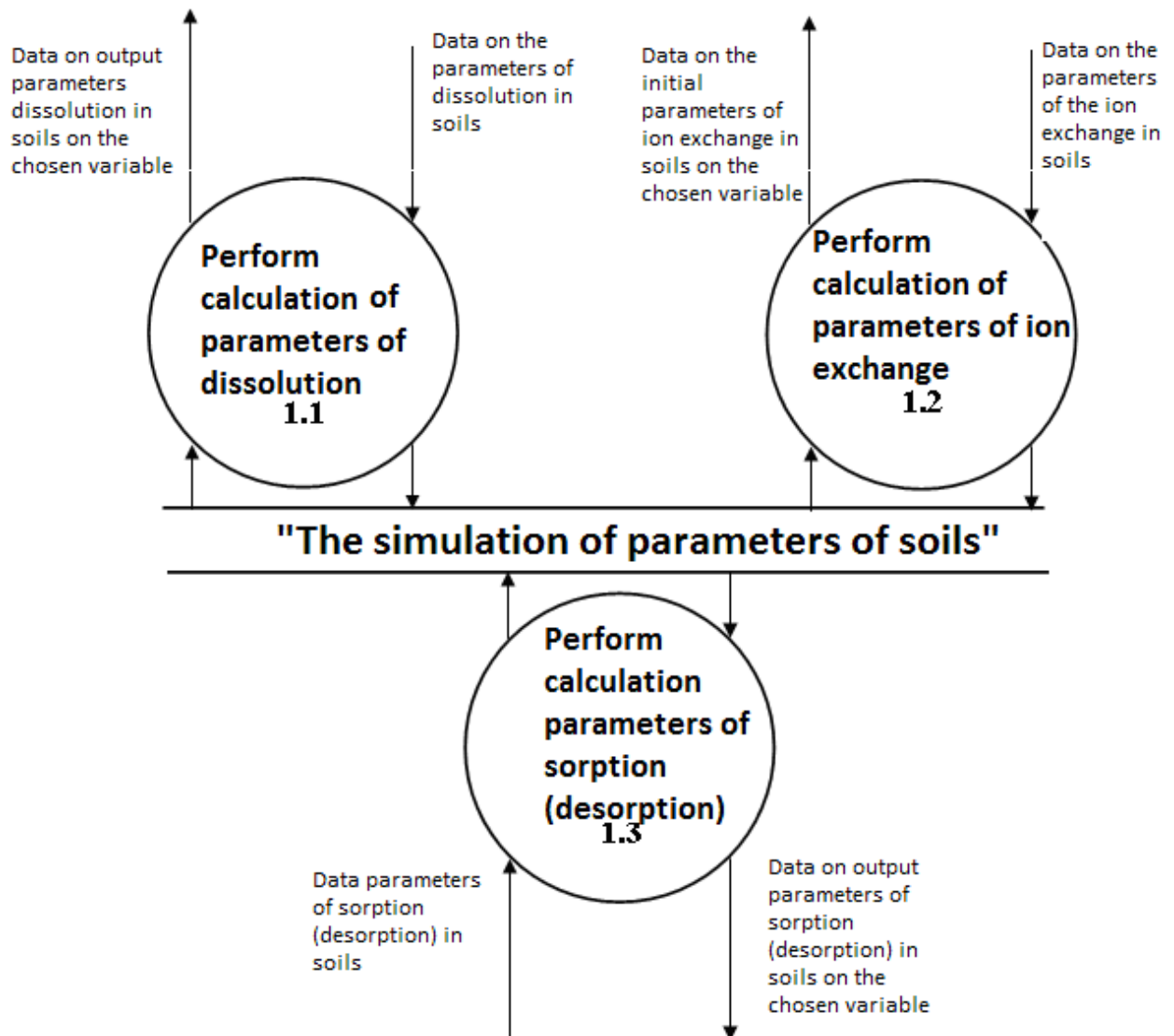


Fig. 5. Context diagram of the second level

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 algorithimized 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.

Исходные данные	Значение
D (плотность почвогрунта)	1300
WP (влажность = полной влагоемкости)	30
WG (гигроскопическая влажность)	10
W0 (влажность, при которой определялась величина CO)	25
W1 (влажность, при которой определялась величина C1)	15
T0 (температура, при которой определялись величины NO, CO и Cк)	293
T1 (температура, при которой определялись величины CP и CZP)	314
TMK (время, через которое после начала растворения определялась величина Cк)	3
CP (концентрация иона в растворе в условиях равновесия)	0,015
CO (концентрация иона в растворе при TM=0)	0,005
CK (концентрация иона в растворе при TM=TMK)	0,0055
C1 (концентрация иона в растворе при влажности W1)	0,008
CZP (концентрация иона в растворе при температуре T1)	0,018
NB (валовое содержание иона в почвогрунте)	0,096
NP (содержание иона в твердой фазе в условиях равновесия)	0
NO (содержание иона в твердой фазе при TM=0)	0

Имитируемый процесс	Выбор
Растворение	<input checked="" type="radio"/>
Ионный обмен	<input type="radio"/>
Сорбция (десорбция)	<input type="radio"/>

по переменной	Выбор
Определение концентрации	<input checked="" type="radio"/>
Определение времени	<input type="radio"/>
Определение температуры	<input type="radio"/>
Определение влажности	<input type="radio"/>

Результаты	Значение
T (Расчётная температура)	298
W (Расчётная влажность)	28
TM (Расчётное время)	30
C (Расчётная концентрация)	0,01023929578

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

Модельовання процесів розчинення, іонного обміну та сорбції (десорбції) в ґрунті

Файл Інформація

Параметри імітації Таблица расчётов Протокол имітації

	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	0,015
COn	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005	0,005
CKn	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055	0,0055
C1n	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008	0,008
CZPn	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018	0,018
NBn	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096	0,096
NPn	0	0	0	0	0	0	0	0	0	0	0	0
NOn	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	0,0102386

Экспорт в Excel Выход

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

Модельовання процесів розчинення, іонного обміну та сорбції (десорбції) в ґрунті

Файл Інформація

Параметри імітації Таблица расчётов Протокол имітації

```

Dn=1300
WPn=30
WGn=10
W0n=25
W1n=15
T0n=293
T1n=303
TMKn=3
CPn=0,015
COn=0,005
CKn=0,0055
C1n=0,008
CZPn=0,018
NBn=0,096
NPn=0
NOn=0
Tn=298
Wn=28
TMn=30
Cn=0,0107400928059554

```

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.

1. Kirillov O. M., Rogalsky F. B., Mykhailyk S. V., Voronenko M. O. *Protection of population and territories from emergency situations of peaceful time.* – Kherson: KHNTU, 2007. – 328 p. 2. Zaychenko D. *Analysis of emergency situations of technogenic and natural character // Emergency situation.* – 2010. – №3. – P.37–38. 3. Guriev S. *State service of disaster medicine as a component of national security of Ukraine / Guriev S., N. Terent'eva // Emergency situation.* – 2010. – №2. – P. 54–56. 4. Goryev L. M., Doroguntsov S. I., Hvesyk M. A. *“Optimization of ecoareas“ Book1.* – Kiev: Naukova dumka, 1997. – 542 s. 5. Gentleman R, Carey V, Huber W, Irizarry R, Dudoit S. / R. Gentleman, V. Carey, W. Huber, R. Irizarry, S. Dudoit // *Bioinformatics and Computational Biology. Solutions Using R and Bioconductor*, 2005. – 473 p. 6. Tchernorutskiy I. G. *Metody optimizatsii v teorii upravleniya.* – SPb.: Piter, 2004. – P. 256.

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\*І. Хомицька, В. Теслюк

Національний університет “Львівська політехніка”,  
\*кафедра прикладної лінгвістики,  
кафедра систем автоматизованого проектування

## МЕТОД СТАТИСТИЧНОГО АНАЛІЗУ ТЕКСТІВ ДРАМАТУРГІЇ Б. ШОУ І РОЗМОВНОГО СТИЛЮ

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Проаналізовано фоностатистичні структури текстів підстилю драматургії та розмовного стилю. Доведено, що середні частоти груп приголосних фонем є критерієм диференціації зіставлених текстів. Побудовано модель визначення ступеня взаємодії текстів художнього (підстиль драматургії) та розмовного стилів. Встановлено ступінь проникнення елементів розмовного стилю в підстиль драматургії художнього стилю за чотирма з восьми груп приголосних фонем, за якими статистичним методом визначено істотні відмінності.

**Ключові слова:** середня частота груп приголосних фонем, фоностатистична структура, позиція фонем в слові.

Phonostatistical structures of the texts of the substyle of drama and colloquial style have been analyzed. Mean frequency of occurrence of groups of consonant phonemes has been proved to be differentiation criterion of the compared texts. A model has been built to determine the degree of interaction of the texts of the belles-lettres (substyle of drama) and colloquial styles. The degree of penetration of elements of the colloquial style into the substyle of drama of the belles-lettres style has been established by four out of eight groups of consonant phonemes by which essential differences have been determined by statistical method.

**Key words:** mean frequency of occurrence of groups of consonant phonemes, phonostatistical structure, position of a phoneme in a word.

## Вступ

Методи математичної статистики є надійним інструментом при розмежуванні текстів мовних різновидів. Особливо це стосується тих випадків, коли функціональні стилі втрачають свою чітко окреслену окремішність і містять достатньо велику кількість спільних елементів. Визначення