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## APPLICATION OF SIMULATION MODELING FOR ASSESSMENT OF ENVIRONMENTAL SAFETY OF SOILS

Об'єктом дослідження є екологічна безпека забруднення ґрунтів промисловим підприємством. Загальний процес геофільтрації розглядається як комплекс окремих фізичних і фізико-хімічних процесів. В ході дослідження розглянуті окремі складові процесу геофільтрації та проведено обґрунтований вибір математичних моделей для їх опису. Одним із проблемних місць є оцінювання впливу типу ґрунту та відповідної цьому типу схеми геофільтрації на загальний результат фільтраційних процесів. Розглянуто класифікацію ґрунтів з точки зору процесів фільтрації, які в них відбуваються. Для різних типів ґрунтів встановлені вагові коефіцієнти впливу окремих процесів, що становлять геофільтрацію. В якості оцінки результатів геофільтрації запропоновано відношення поточної концентрації забруднювача до його фонові концентрації. Запропоновано методіку визначення показників ефективності очищення, заснована на імітаційному експерименті. Розроблено алгоритм проведення імітаційного експерименту на комплексі моделей з урахуванням встановлених коефіцієнтів і проведено 10000 його реалізацій. За результатами імітаційного експерименту визначено величини, що дозволяють судити про якість геофільтрації:

– інтервальна оцінка ступеня очищення;

– висота ґрунтового шару, яка забезпечує максимально можливу ступінь очищення та ймовірності повного очищення від забруднювача під час проходження через шар ґрунту для всіх розглянутих ґрунтів.

Запропоновано розглядати ризик проникнення забруднювача в підземні води через шар ґрунту та встановлено шкалу оцінювання цього ризику на основі шкали бажаності Харрінгтона. Для всіх розглянутих типів ґрунтів оцінено ризик проникнення забруднень у випадках, коли початкова концентрація забруднювача перевищує фонову в три, п'ять і десять разів.

Завдяки цьому забезпечується можливість отримання значень показників ефективності геофільтрації в залежності від початкової концентрації забруднювача з урахуванням типу ґрунту. Ці показники рекомендується враховувати під час проектування місць розміщення потенційно небезпечних об'єктів і виробництв.

**Ключові слова:** екологічна безпека, забруднення ґрунтів, геофільтрація, імітаційний експеримент, ступеня очищення.

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### 1. Introduction

The increase in anthropogenic influence, which is due to technological progress, leads to an increasingly noticeable change in the state of the environment, and most of them have a negative effect on all life on the planet.

Man-made environmental impacts in modern conditions are so great that catastrophic changes in climatic, geological, tectonic and seismic conditions are possible, as well as the occurrence of global pollution, etc. And, as a result, changes in the development of ecosystems, biological diversity of living conditions of people and their health, the change in the sustainability of technological activities.

The fundamentals of the general concept of influence on environmental elements, in particular, on soils and groundwater, are presented in [1] at the end of the last century. In connection with the intensive development of industrial and urban areas, the scales of the manifestation of the negative influence of processes and phenomena, as well as the amount of damage to the soil, are expanding. As a result of this, a problem arises in studying the processes

of influence and changes that arise in the territories for the development of protective measures with maximum regard for varieties of natural and man-made factors.

Thus, the study of the impact of industrial facilities on the environment is relevant. For this, it is necessary to create such methods of mathematical modeling that will make it possible to reduce the technological load on the components of the environment.

### 2. The object of research and its technological audit

*The object of research* is environmental safety of soil pollution by an industrial enterprise.

Currently, passivity in the problem of resolving environmental safety issues, and soils in particular, for humanity can cause irreversible processes. Human activity is inextricably linked with an increase in the load of pollutants on the soil of industrial ecological systems. A high degree of pollution of atmospheric air and water leads to the accumulation of pollutants in the soil. Moreover,

this is also observed during the normal operation of enterprises, especially the chemical industry. Only monitoring can't solve the problem of environmental safety of territories; forecasting methods are needed for informed decision-making. For an objective solution to the problem of reducing the man-made load, it is necessary to estimate the level of distribution of the pollutant in the soil in advance quantitatively.

### 3. The aim and objectives of research

*The aim of research* is to determine all the features of the process of soil pollution by an industrial enterprise.

To achieve this aim it is necessary to perform the following objectives:

1. To highlight the mathematical models, which best describe the physicochemical processes in soils.

2. To separate soil types of Ukraine with different geofiltration conditions in a separate classification.

3. To determine the ratio of mathematical models to soil types.

4. To determine the level of influence of the industrial enterprise on the soil layer.

### 4. Research of existing solutions of the problem

The authors analyze a number of works devoted to the assessment and modeling of filtering processes of pollutants coming through the soil layer. The fundamental work in this direction, according to the authors, is the work [2]. In this work, a number of models of the process of mass transfer of soluble substances when moving through a soil layer are proposed. The generalized geofiltration model proposed by the author of this work is a functional differential equation of the second order in partial derivatives. The author does not set the task of obtaining a generalized solution to this equation, since the functions introduced into it strongly depend on the conditions of the process. However, the paper considers three main options for solving this equation – for the averaged and variable filtration rates and in the case of convective diffusion. However, the problems of transferring the obtained simulation results to real soils remained unsolved, since the author does not give recommendations on the criteria for the applicability of one or another solution to the model. In addition, only the convective diffusion process is considered in the work, at the same time, other physicochemical processes also have a significant effect on geofiltration.

In continuation of the aforementioned work, it is proposed in [3] to consider filtration in the soil, based on mass transfer processes occurring at the phase boundary during the motion of a Newtonian fluid through cylindrical tubes. The author of [2] suggests considering such a formal structure as ideal soil. To describe the filtration process, the author of [3] recommends using the dependence of the filtration rate based on the Leverett function, which approximately corresponds to low and high filtration rates. However, the assumption about the movement of the pollutant in the soil in the capillary mode is not accurate enough, and the author's conclusion about the need to clarify Darcy's law is general.

In [4], mathematical modeling of the process of saline water purification with an initial salt concentration of

15 g/l when passing through the soil layer is considered. This takes into account the partial accumulation of salts and the establishment in the soil of the concentration of salts, which has the essence of the background. The mathematical model of the filtration process proposed by the authors has the form of a system of algebraic equations and second-order differential equations in partial derivatives. However, the authors do not take into account the difference in the composition of soils of different types. In addition, the authors did not complicate the model by introducing into it the whole complex of processes occurring in soils during filtration. At the same time, it seems appropriate for the authors to use a simulation experiment to study filtration processes in the soil, since finding a generalized solution to a system of mathematical models is extremely difficult.

The authors of [5] proposed a mathematical model of the mass transfer process in saturated and unsaturated porous media under isothermal conditions to simulate the spread of contaminants in the soil. The model is a system of differential equations of the first and second orders in partial derivatives. The undoubted advantage of the proposed model is the consideration of the movement of the pollutant not only in the vertical, but also in the horizontal directions. The result of the solution of the model is the field of pollutant concentrations in the soil. However, the authors focus their work only on the processes of mass transfer and mass transfer, although geofiltration is not limited to only these processes. Thus, the problems of taking into account the influence of the processes of mechanical, chemical, etc., components of geofiltration remained unresolved. It should be noted that the authors also failed to obtain a generalized solution to their proposed model due to its rather high complexity. The solution proposed by the authors is obtained by numerical methods.

In the development of research [2], in the work [6], performed with the participation of the authors, it is proposed to take into account the physicochemical characteristics of the soil to build a model of the geofiltration process. In addition to the already mentioned convective diffusion coefficient, the active porosity of the medium and bulk density is introduced into the model. The obtained results more adequately describe the experimental data of the filtration process in real soil. At the same time, the issues of the influence of other physical and chemical parameters of the soil remained unresolved.

In [7], the authors present the results of modeling the spread of pollution in sandy soils. As pollutants, the combined composition of the municipal waste dump is considered. The undoubted advantage of the work is the form of the model accepted by the author – linear, power-law and quadratic regression equations. These equations describe the relationship between the masses of the introduced and filtered pollutant per unit area of soil. Despite the use of simple mathematical dependencies, the obtained simulation results correlate with real results with a coefficient of 0.98±0.99. The authors point out the possibility of adapting the regression equations it proposed for other soil compositions other than those considered in the work of sandy soils and various types of pollution, but the adaptation itself was not carried out.

It should also be noted [8], in which the authors propose a mathematical model of the inverse problem of removing contaminants from the soil by washing contaminated, in

this case saline soils. The models proposed by the authors are based on fairly simple structural equations of chemical kinetics. The authors propose to consider the process of removing contaminants as a first-order chemical reaction. However, other types of interactions between pollutants and the soil layer remained unexamined. The authors' assumption of the first order of interaction when washing with water particles of a solid substance – soil – seems rather crude.

A more thorough attempt to develop a mathematical model of the processes occurring during leaching of the soil, as well as desalination and purification of soils from pollutants, is made in [9]. The authors propose a model of the dynamics of the locally non-equilibrium in time process of convective diffusion of soluble substances under the conditions of plane-vertical stationary filtration of groundwater, taking into account the presence of interphase mass transfer. The authors obtain integral differential models of the non-equilibrium convective-diffusion process in a porous medium under mass transfer conditions. Based on the developed models, the authors perform computational experiments and computer simulations, the results of which show the propagation front of contaminants in soils taking into account mass transfer. However, the authors do not take into account the differences between the types of soils that are to be washed, which would undoubtedly make adjustments to the processes occurring in the soil.

In [10], the authors develop a facility for studying the penetration of pollutants – heavy metals generated as a result of fuel combustion in a car engine, into the ground. Based on theoretical and experimental studies, they propose a physical and mathematical model of the penetration of these pollutants into the soil and determined the maximum depth of their penetration. However, the mathematical model proposed by the authors is actually an equation of the material balance of the process. Also, the authors do not take into account the background concentrations of the studied pollutants in the study, the measurement of which made significant adjustments to the results obtained by the authors, since the error in the concentration changes (reaching 10 %, in one case 15 %) significantly exceeds the background concentration of pollutants.

It is also possible separately to distinguish works in which specific features of the movement of moisture in the soil are noted [11, 12]. And studies in which several groups of specific phenomena of soil moisture transfer are distinguished:

- fast transfer along the «leading» pore spaces and further exchange with stagnant zones;
- uneven movement of soil moisture associated with variability of soil properties;
- movement along macropores [13];
- formation of individual water channels, lines of preferential flow [14].

After analyzing the results of studies on the problems of filtering contaminants when passing through a soil layer, the authors came to the conclusion that it is difficult to describe this process using one mathematical model. The geofiltration process is complex and various physical, physico-chemical and chemical processes take part in it. Therefore, it is advisable to conduct studies of the filtration properties of soils on the basis of models of individual processes, taking into account the relative contribution of such processes to the overall geofiltration process for various types of soils.

## 5. Methods of research

To solve the problems, the most promising are the following of the above models:

- 1) a model for assessing soil pollution taking into account a chemical reaction in the filtering process [15–17];
- 2) a model for assessing soil pollution taking into account the features of the soil layer [6];
- 3) a model for assessing soil pollution taking into account mass transfer processes [2];
- 4) a model for assessing soil pollution taking into account mass transfer processes: with uniform sorption [2];
- 5) a model for assessing soil pollution taking into account mass transfer processes: with uneven irreversible sorption [2];
- 6) a model for assessing soil pollution taking into account mass transfer processes: during crystallization or dissolution of rock components in wastewater [2].

## 6. Research results

**6.1. Consideration of soil features during a simulation experiment.** The types of soils with different geofiltration conditions are presented in [1].

Systematization of data on geological and hydrogeological conditions makes it possible to distinguish 4 areas of filtration schemes and 9 regions in their composition in Ukraine:

1. Aeolian-deluvial soils of the loess complex:
  - 1.1. With the presence at the base of the cover deposits of relative water resistance.
  - 1.2. Without the presence of relative waterproofing at the base of the cover sediments.
2. Alluvial deposits of river terraces:
  - 2.1. With the presence at the base of the cover deposits of relative water resistance.
  - 2.2. Without the presence of relative waterproofing at the base of the cover sediments.
3. Modern marine sediments:
  - 3.1. With the presence at the base of the cover deposits of relative water resistance.
  - 3.2. Without the presence of relative waterproofing at the base of the cover sediments.
4. Fissured rock and semi-rock:
  - 4.1. With the presence of integumentary aeolian-deluvial deposits.
  - 4.2. With the presence of integumentary alluvial deposits.
  - 4.3. With the presence of aeolian-deluvial deposits, destroyed rock and semi-rock.

According to the classification, which is proposed based on the study [1], the aeolian-deluvial soils of the loess complex include: aeolian-deluvial soils of the loess complex, continental red-brown Pliocene-Lower Quaternary clays and/or green-gray sea clays of the Neogene age and sand-clay deposits of river and sea terraces with a predominance of the first species. Depending on the types and composition of the soil, certain physical and chemical processes in the soils prevail, which can significantly affect the filtration properties of the soil layer. In this type of soil, in connection with the ratio of its composition, the processes prevail in which it is necessary to take into account the features of the soil layer to a greater extent, as well as processes in which the chemical reaction and mass transfer are taken into account. In this regard, to

assess soil pollution, processes are taken into account in the following ratio:

- assessment taking into account the features of the soil layer during the filtration process will be 35–40 %;
- assessment taking into account mass transfer processes in 15–25 %;
- assessment taking into account the chemical reaction in the filtration process will be 15–20 %;
- assessment taking into account mass transfer processes: with uniform sorption of 7–20 %, with uneven irreversible sorption of 5–10 %, with crystallization or dissolution of rock components in wastewater at 0–5 %.

Let's assume that these ratios of filtration processes will correspond to the fraction that describes their models in the general calculation. For the indicated type and other soils in accordance with the classification, the ratio of the models is shown in Table 1.

**Table 1**

Matrix of relations of mathematical models to soil types

Soil type	Impact assessment boundary	Model serial number					
		1	2	3	4	5	6
1.1	lower	0.15	0.35	0.15	0.07	0.05	0
	top	0.2	0.4	0.25	0.2	0.1	0.05
1.2	lower	0.2	0.28	0.09	0.15	0.05	0
	top	0.25	0.35	0.2	0.25	0.1	0.05
2.1	lower	0.3	0.2	0.1	0.1	0.05	0
	top	0.4	0.3	0.2	0.15	0.1	0.05
2.2	lower	0.3	0.25	0.1	0.1	0.05	0
	top	0.35	0.3	0.2	0.15	0.1	0.05
3.1	lower	0.15	0.3	0.17	0.05	0.11	0
	top	0.2	0.35	0.25	0.1	0.25	0.05
3.2	lower	0.15	0.3	0.16	0.07	0.08	0
	top	0.2	0.4	0.25	0.12	0.16	0.05
4.1	lower	0.1	0.1	0.05	0.05	0.05	0.4
	top	0.15	0.2	0.1	0.1	0.1	0.5
4.2	lower	0.05	0.15	0.07	0.05	0.05	0.4
	top	0.1	0.2	0.13	0.14	0.12	0.5
4.3	lower	0.1	0	0.05	0.07	0.07	0.5
	top	0.2	0	0.1	0.13	0.15	0.6

**6.2. Determination of interval assessment of the degree of possible purification during geofiltration.** Since the accepted assessment of the degree of influence of individual processes and their corresponding models on the result of geofiltration are interval in nature, as can be seen from the Table 1, an assessment of the degree of possible purification determined on the basis of a group of models will also be interval. To determine it, let's use the following algorithm. At the first step, let's simulate the concentration of the pollutant for each of the models selected in section 5 separately. Let's calculate based on the depth of the soil layer in increments of 0.1 m until the concentration calculated by all selected models reaches the background. Thus, the maximum layer depth ( $D_{max}$ ) will be found. The calculation showed that for the initial concentration of the pollutant, exceeding the background depth by 3 times, this depth is 2.9 m, 5 times – 4.9 m, 10 times – 11.0 m.

In the second step, let's calculate the purification degree at each point in depth for all selected models.

The purification degree is calculated as the ratio of the current concentration to the background. At the third step, the found purification degrees are summarized taking into account the degree of influence of individual models (Table 1). Thus, the top and lower boundaries of the purification degree at each depth are determined. If, as a result of addition, the obtained value exceeds one, it is replaced by one.

Table 2 shows the results of calculations by the described algorithm – the depth of achieving a single purification degree at the upper boundary ( $D_1$ ) and the maximum purification degree at the lower boundary ( $q_{max}$ ).

**Table 2**

Depths at which a purification degree is achieved, equal to one at the top boundary ( $D_1$ ) and the maximum possible purification degree at the lower boundary ( $q_{max}$ ) in soils of different types

Soil type	$C_b \times 3$		$C_b \times 3$		$C_b \times 3$	
	$D_1$	$q_{max}$	$D_1$	$q_{max}$	$D_1$	$q_{max}$
1.1	1.4	0.833	3.1	0.833	9.1	0.833
1.2	1.5	0.833	3.5	0.833	9.6	0.833
2.1	1.7	0.833	3.9	0.833	9.9	0.833
2.2	1.8	0.87	4.1	0.87	10.1	0.87
3.1	1.5	0.833	3.1	0.833	9.1	0.833
3.2	1.4	0.847	2.9	0.847	9	0.847
4.1	1.5	0.87	2.5	0.87	7.9	0.87
4.2	1.5	0.84	2.6	0.84	8	0.84
4.3	1.7	0.847	2.7	0.847	8.4	0.847

**6.3. Simulation experiment to determine the probability of the maximum possible purification.** To determine the probability of the maximum possible purification, which will be interpreted as achieving a pollutant concentration equal to the background, it is proposed to conduct a simulation experiment. The implementation of a single experiment is as follows. Let's accept that the degree of influence of each of the purification processes in the soil and, as follows from the above accepted assumption, the degree of participation of the model, is a random variable. The distribution law of this quantity is uniform in the interval equal to the accepted interval from the Table 3. According to the indicated law, let's draw these random variables and obtain their point values. When drawing, let's take into account that the sum of all the values played is equal to one.

**Table 3**

Depths at which the maximum probability ( $P_{DMP}$ ) of the maximum possible purification in soils of different types is achieved

Soil type	$P_{DMP}$	Depth, m		
		$C_b \times 3$	$C_b \times 5$	$C_b \times 10$
1.1	0.610	1.3	3.7	9.5
1.2	0.600	1.8	4.1	9.8
2.1	0.660	1.7	4.2	10
2.2	0.714	1.9	4.3	10.4
3.1	0.570	1.8	3.7	9.8
3.2	0.716	1.6	3.6	9.7
4.1	0.832	1.6	2.6	8.9
4.2	0.634	1.6	2.5	7.9
4.3	0.616	1.7	3.2	9.3

The next step is to calculate the concentration of pollutants in the soil for all models, taking into account the obtained point values of the degrees of their influence. The calculation is carried out for each depth from the soil surface to that found in Subsection 6.1 with an accepted step of 0.1 m. If the obtained concentration at a given depth does not exceed the background concentration of pollution in the soil (with a rounding error), let's recognize a single experiment for this depths successful, otherwise – not successful.

Based on the results of implementing a sufficiently large number of single experiments, the relative frequency of successful experiments for each depth can be calculated. According to the law of large numbers, with an increase in the number of experiments, this relative frequency will tend to the probability of complete purification with an increase in the number of single experiments. In this study, 10,000 such experiments were implemented. The results of the calculation of the relative frequency (statistical probability) of the maximum possible purification ( $P_{MBO}$ ) are given in Table 3.

As can be seen from the Table 3, the statistical probability of the maximum possible purification does not depend (up to the results of a simulation experiment) on the initial concentration of the pollutant. Only the depth at which the maximum possible purification is achieved depends on the initial concentration.

**6.4. Determination of the risk of contamination through the soil.** Let's establish the acceptability of purification based on the magnitude of the risk of incomplete purification. Let's take such a risk as  $1-P_{DMP}$  and set its marks in accordance with the Harrington desirability scale [12], Table 4.

**Table 4**  
Acceptability grade

$1-P_{DMP}$	Acceptability grade
0÷0.2	Definitely acceptable
0.2÷0.37	Acceptable
0.37÷0.63	Conditionally acceptable
0.63÷0.8	Unacceptable
0.8÷1	Definitely unacceptable

The acceptability of the risk of contaminant penetration through the soil layer depending on the depth of this layer is summarized in Tables 5, 6.

**Table 5**  
The risk of pollution penetration through the soil layer (initial concentration three times higher than the background)

Soil type	Depth, m, at which the risk of penetration:		
	definitely unacceptable	conditionally acceptable	definitely acceptable
1.1	<2.0	>2.2	not achieved
1.2	<2.1	>2.3	not achieved
2.1	<2.1	2.2–2.4	not achieved
2.2	<2.1	2.2–2.3	not achieved
3.1	<2.0	>2.3	not achieved
3.2	<2.0	2.2–2.3	not achieved
4.1	<1.8	2.0–2.1	>2.4
4.2	<1.8	2.0–2.3	not achieved
4.3	<2.1	2.2–2.4	not achieved

**Table 6**

The risk of contamination through the soil layer (the initial concentration exceeds the background tenfold)

Soil type	Depth, m, at which the risk of penetration:		
	definitely unacceptable	conditionally acceptable	definitely acceptable
1.1	<10.3	>10.5	not achieved
1.2	<10.4	>10.6	not achieved
2.1	<10.5	10.7–10.8	not achieved
2.2	<10.5	10.7–10.8	not achieved
3.1	<10.4	>10.7	not achieved
3.2	<10.2	10.5–10.7	not achieved
4.1	<9.8	10.1–10.4	>10.8
4.2	<9.8	10.1–10.7	not achieved
4.3	<10.2	10.5–16.4	not achieved

Based on the results of the simulation experiment, it is possible to draw the following conclusions:

- for aeolian-deluvial soils of the forest complex of type 1.1, conditionally acceptable purification is achieved at a depth of 1.3, 3.7, and 9.5 m for 3 different experiments, respectively;
- for aeolian-deluvial soils of a forest complex of type 1.2, conditionally acceptable purification is achieved at a depth of 1.8, 3.6 and 9.8 m, respectively;
- for modern marine sediments of type 3.1, conditionally acceptable purification is achieved at a depth of 1.8, 3.7 and 9.8 m, respectively;
- for fractured rock and semi-rock type 4.3, conditionally acceptable purification is achieved at a depth of 1.7, 3.2 and 9.3 m, respectively;
- for alluvial deposits of river terraces of type 2.1 acceptable purification is achieved at a depth of 1.7, 4.2 and 10 m;
- for alluvial deposits of river terraces of type 2.2, acceptable purification is achieved at a depth of 1.9, 4.3 and 10.4 m;
- for modern marine sediments of type 3.2 acceptable purification is achieved at a depth of 1.6, 3.6 and 9.7 m;
- for fractured rock and semi-rock type 4.2, acceptable purification is achieved at a depth of 1.6, 2.5 and 7.9 m;
- for fractured rock and semi-rock rocks of type 4.1, unconditionally acceptable purification is achieved at a depth of 1.6, 2.6 and 8.9 m;
- for rock types 1.1, 1.2, 3.1 and 4.3, acceptable purification in the territory can't be achieved.

## 7. SWOT analysis of research results

**Strengths.** The main strength of the proposed methodology is that at the moment there are no such methods that can allow to assess the risk level of the influence of an industrial enterprise on the soil by the height of its layer.

**Weaknesses.** The main weakness of the proposed methodology is that the matrix of the ratios of mathematical models to soil types (Table 1) is suitable for the corresponding soil types with the classification presented in Section 6.1. And when using the methodology for other types of soils, it will be necessary to introduce a correlation matrix that better describes the physical processes that occur in it.

*Opportunities.* The problem of predicting the anthropogenic impact on the state of the soil layer is nowhere sufficiently integrated into the decision-making system. In this regard, the application of this technique will allow: to actually assess the level of negative impact on the soil, as well as decide on its consequences.

*Threats.* The application of this technique does not require separate costs for its implementation, and it is necessary to know the list of substances that enter the soil and their concentration. In this regard, the introduction and use of it in enterprises does not pose any threats.

## 8. Conclusions

1. Six mathematical models have been identified that best describe the physical and chemical processes in the soil layer.

2. The Ukrainian soil is classified to describe the distribution of pollutants with a fluid flow in the soil layer, depending on its different geofiltration conditions.

3. To solve the problem of determining the level of influence of enterprises on the soil layer, a matrix of relations of mathematical models to soil types is created, which takes into account the specifics of the composition of the soil layer and the physicochemical processes in it.

4. To determine the level of influence of an industrial enterprise on soils, interval estimates of the degree of possible purification for different types of soils were found. It also found the probability of the maximum possible purification and the depth at which it is achieved for different types of soils. As a result, this allows to determine the risk of contaminants penetrating through the soil layer for different types of soils.

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