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BIOCOLMATION AND THE FINITE ELEMENT MODELING OF ITS INFLUENCE ON CHANGES IN THE HEAD DROP IN A GEOBARRIER

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The influence of the biocolmation of the geobarrier for organic waste storage on the values of head drops has been investigated. A mathematical model of filtration of organic substances taking into consideration the biocolmation effect was formed. The mathematical model contains the equation of filtration under conditions of variable porosity. In addition, the mathematical model includes the equation of transfer of organic chemical substances in pore fluid and the equation of dynamics in bacteria biomass in a porous medium based on the Monod equation. The problem in the region with a thin inclusion was solved by the method of finite elements. The schematic algorithm of finding an approximate solution of the boundary problem, including the scheme of discretization over time, is presented. Numerical experiments were conducted with an analysis of their results. In particular, the tables have been given of the values of heads and their drops on inclusions when biocolmation is neglected and the values of heads and their drops on inclusions while taking into account biocolmation at specific moments of time. The numerical experiments showed that the existence of microorganisms in soil pores significantly influences the values of heads at the top and at the bottom of a geobarrier. In particular, relative changes in head drops, in comparison with the case of disregarding the influence of microorganisms, can reach 54.8 % towards an increase. Such differences, in turn, lead to a change in the estimation calculations of the propagation of waste storage contamination into groundwater. They can also cause negative changes in the stressed-strained state of a soil array in the vicinity of a geobarrier as a type of a thin inclusion and lead to the intensification of shear processes. At the same time, due to the nonlinearity of influences and complex interdependence among processes, it is not possible to predict such values and their differences without computer simulation and mathematical modeling

Keywords: biocolmation, organic waste, geobarrier, a finite element method, model of bacteria development

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1. Introduction

The development of industrial production and major cities actualizes the problem of today – waste storage and recycling. The design and construction of waste storage should perform the main function – to minimize the spreading of harmful substances from storage to the environment. One of the design solutions to this problem is the use of so-called geobarriers in soil storages [1, 2]. A geobarrier is a thin layer of natural or (and) synthetic material, which (layer) has pronounced non-penetration properties for harmful substances. A change in the physical-chemical protective properties of the geobarrier material due to the influence of external factors remains a relevant direction of scientific research, as it is related to the safety of life and health of people.

In the presence of organic wastes in the storage, one of the factors of influence on the geobarrier parameters is the development of microorganisms, and, as a consequence, biocolmation. Biocolmation may be the cause of changes in hydrological parameters of the porous material of a geobarrier. This, in turn, leads to changes in estimation calculations of contamination propagation from waste storage to the groundwater. At the same time, in virtue of non-linearity of the influences and complex interdependence of processes, it is impossible to predict the values of the amount of harmful substances that got to the environment through a geobarrier without computer simulation and mathematical modeling.

2. Literature review and problem statement

In paper [4], it was proposed to take into account a change in the hydrological parameters of geobarriers in the bases of waste storage in case of the influence of inorganic chemical substances and temperature. It was mathematically expressed in the modification of the conjugation conditions for humidity, contamination concentration and temperature in comparison with the classical case. In addition, in paper [5], the effect of chemical suffusion of the geobarrier material and its (material) possible structural changes under the influence of aggressive chemical solutions of inorganic origin were theoretically taken into consideration. In studies [3, 6], the method of finite elements was applied to the numerical solution of the corresponding boundary problems with modified conjugation conditions. Using the example of numerical experiments, it was shown that in some cases it is not permissible to neglect nonlinear dependences of physical-chemical parameters of the material of thin inclusions, and consequently – modification of conjugation conditions.

However, these works do not explore the peculiarities of spreading organic substances from storages of domestic wastes, as a rule. One of these features is the development of microorganisms (which is fundamentally impossible in the presence of inorganic chemical waste) and, consequently, biocolmation of the porous material of a geobarrier. We aim to consider this factor of influence by constructing an appropriate mathematical model and its numerical research. While the main components of the mathematical model concerning the motion of the pore fluid, the contamination propagation, modification of conjugation conditions at a change in the properties of the material of a geobarrier are explored in research, for example, in papers [6] or [4], the development of microorganisms in the porous medium requires special attention.

The first step in this direction is an overview of available scientific research, which can be conditionally divided into two subgroups. The first one relates to the effect of microorganisms on the characteristics of porous media. The aim of such an overview is to show the existing scientific contribution at the level of field experiments, which once again emphasizes the relevance of the research and provides the grounds for mathematical and computer modeling. The second group refers to proper mathematical models of development and propagation of microorganisms in media, including porous ones.

Paper [7] provides a thorough overview of studies into the mechanisms of the biocolmation of porous media. In relation to mathematical modeling of biocolmation, its consequences, such as a decrease in filtration factor of a porous medium, were studied. The authors analyzed the analytical formulas for filtration factor, well-known in the scientific literature, however, mathematical models of the dynamic change of microorganisms in the porous medium were not considered and explored.

Paper [8] describes the field experiments on studying the influence of biocolmation on hydroconductivity of sandy soil. The author presented a thorough analysis of the known dependences of filtration factor on a change in porosity as a result of germs activity. Based on a comparison of his own experiments with the known ones, the author concluded that a decrease in hydroconductivity, in this case, is described by the models of colonies development, rather than the models based on biofilms. However, the author did not go further in his research – application of the obtained dependences in mathematical models.

The important problem of denitrification in agricultural production was studied in paper [9]. During the experiments, as a part of general dynamics, the development of microbes as one of the factors of denitrification (neutralization and decomposition of nitrates) was studied. This research shows that bio-processes in porous media, including the development of microorganisms, are important in different problems and their exploration is a relevant task of today. The results of research [10] also prove it. These studies can be applied to research into the problems of waste neutralization at their propagation from storage. However, it was not done in the above papers.

The effect of microbial development on the filtration factor of a mixture of sludge and bentonite (three samples with 0 %, 5 %, 10 % of bentonite content) was studied in article [11]. When studying the filtration of nutrients solution on day 540 from the beginning of the research, the filtration factor of all soil samples decreased almost by an order of magnitude. If researchers subsequently replaced nutrients with antibiotics and antifungal drugs, on day 720 (180 days after the replacement), the filtration factor acquired the values characteristic to the beginning of the experiment. In the article, the results of experiments were compared with the known theoretical dependences of other researchers concerning the influence of biocolmation on filtration factor and good match both in qualitative and quantitative terms was obtained. The researchers see the benefits of their research in the fact that it shows the possibility of influencing and controlling in terms of hydro-conductivity and improving the efficiency of geobarriers of waste storage. However, the researchers did not apply the obtained results to the improvement of mathematical and computer models of the relevant processes.

Article [12] can be divided into two parts. In the first part, the authors perform a theoretical assessment of the impact of biomass existence in the porous medium on a change in permeability (in the sense of fluid filtration) of the mentioned medium. In particular, the authors used the approaches based on functional dependences by van Genuchten, on functional dependences by Brooks-Corey. And both cases gave the same result.

$$\frac{\bar{k}_b}{\bar{k}_0}=\left(1-\frac{n^f}{n_0}\right)^{19/6},$$

where $\bar{k}_0$, $\bar{k}_b$ are the factors of permeability of «clean» porous medium and the medium under the influence of germs activity; n^f is the volume fraction of the biomass; n_0 is the soil porosity. The authors termed the proposed approach a «microscopic approach». The other part of the article compares the obtained dependences with the models based on biofilm development. The studies showed the coincidence of results with relatively high accuracy. The mathematical model of the dynamics of microorganisms in a porous medium, proposed by the authors, includes the following three main equations. The first is the differential equation of nutrients propagation. The second is the differential equation for microbe propagation in the pore fluid. The third is a differential equation that describes the dynamics of a change in the number of microorganisms, absorbed by the skeleton of the porous medium. However, the porous medium considered by the authors is homogeneous and does not contain thin inclusions.

In paper [13], the field experiments revealed that the magnitude of the filtration factor of soil samples decreased by order of magnitude 12 days after the beginning of tests on the filtration of organic substances. Using the obtained values, the authors performed finite-element estimation calculations using a one-dimensional mathematical model of contamination propagation. The time of concentration breakthrough beyond the protective geobarrier of waste storage was studied. At the factor of clean water filtration, such breakthrough occurs after 25 years, and at the values of filtration factor that are by one order of magnitude lower – after 90 years. However, the considered model is linear, it was explored at various constant values of filtration factor, that is, its dynamic change in the process of numerical computer experiments is impossible. In addition, the medium was considered without the existence of fine inhomogeneous inclusions in it.

The authors of article [14] notice that the Monod model of microbe growth historically became the first model of dynamics of microorganisms:

$$\frac{\mathrm{d}B}{\mathrm{d}t} = \mu B = \mu_{\max} B \frac{S}{k_s + S},$$

where, according to the authors' designations and definitions, B is the biomass, $\mu_{\max}$ is the specific growth rate, S is the substrate concentration, and k_s is the Monod constant of semi-saturation, that is, the substrate concentration when $\mu = 0.5\mu_{\max}$. The specified point model has many classifications that include the existence of several types of microorganisms, their interaction, the existence of biochemical reactions, etc.

However, the model based on the classical Monod equation has a drawback – the biomass of microorganisms in the presence of a favorable medium can increase up to infinity. In paper [15], it was emphasized that one of the ways to eliminate this drawback is to use a logistic equation of development of microorganisms:

$$\frac{\mathrm{d}c_{bac}}{\mathrm{d}t} = \mu_{bac} c_{bac} \left(1 - \frac{c_{bac}}{c_{bac}^{\max}}\right),$$

where c_{bac} is the biomass of microorganisms, $\mu_{\max}$ is the growth factor, $c_{bac}^{\max}$ is the maximum permissible biomass of microorganisms in a unit of volume of the medium (the author's designations).

The authors of article [16] proposed the so-called TBC-model of propagation of organic substances in the porous medium. The essence of the model is that the elementary volume of a porous medium conditionally consists of three phases: liquid phase; solid phase; and biophase. In particular, a known equation of elastic filtration was used as the filtration equation:

$$\nabla \cdot \left(k_g \nabla h\right) = s_0 \frac{\partial h}{\partial t} - w,$$

where s_0 is the storage factor; w is the source; k_f is the filtration factor; h is the piezometric drop. To change the concentration of the solution in pore water, the equation of the parabolic type was used:

$$\frac{\partial c_{mob}}{\partial t} = -\nabla \cdot \left(u c_{mob}\right) + \nabla \cdot \left(D \nabla c_{mob}\right) + r,$$

where c_{mob} is the concentration of the dissolved substance in aqueous phase; D is the dispersed tensor, including molecular diffusion; $u = v/n$ is the velocity of fluid motion; v is the filtration rate; n is the soil porosity; r is the function of sourced and drains of chemical substances. The exchange of dissolved substances between the water phase and the biophase is modeled with the help of [16]:

$$\frac{\partial c_{bio}}{\partial t} = -\frac{\lambda}{n_{bio}} \left(c_{bio} - c_{mob}\right),$$

and

$$\frac{\partial c_{mob}}{\partial t} = \frac{\lambda}{n} \left(c_{bio} - c_{mob}\right),$$

where c_{bio} is the concentration of the dissolved substance in the biophase; λ is the parameter of the changed course.

The specific volume of biophase is n_{bio}. It is assumed that biomass X changes according to the Monod equation:

$$\frac{\partial X}{\partial t} = \mu_{\max} X \prod_i \frac{c_{bioi}}{k_i + c_{bioi}} - \mu_{dec} X.$$

However, the proposed general models are not applicable to studying the processes in non-homogeneous media when there are geobarriers.

The author of article [17] notes that the biomass influences filtration processes in the soil due to a change in porosity, and hence it influences filtration factor. In the article, the author made a review of such dependences of filtration factor on porosity, known from scientific sources. However, the author did not apply the above-mentioned dependences in mathematical models for moisture transfer and filtration and did not evaluate the impact of such dependences on changes in heads and humidity in soil.

The model of biocolmation of a porous medium, developed and studied by the authors of article [18], includes:

1) the equation of mass transfer in a porous medium:

$$\frac{\partial c_{mob}}{\partial t} = \frac{\partial}{\partial y}\left(D_L \frac{\partial c_{mob}}{\partial y}\right) - v \frac{\partial c_{mob}}{\partial y} + s,$$

where c_{mob} is the concentration of a dissolved substance in the moving phase; D_L is the coefficient of longitudinal dispersion; v is the average porous velocity; t is the time; y is the distance; s represents changes in the concentration of the moving phase of the types due to the chemical or biochemical reaction in a porous media;

2) the model of bacteria growth:

$$\frac{\partial X}{\partial t} = v_{\max} \frac{c_1}{k_{s1} + c_1} \cdot \frac{c_2}{k_{s2} + c_2} X,$$

where $v_{\max}$ is the maximum growth rate; c_1 is the concentration of basic substrate in biophases; c_2 is the concentration of secondary substrate in biophases; k_{s1} is the constant of semi-saturation of the basic substrate; k_{s2} is the constant of semi-saturation of the secondary substrate; X is the general concentration of bacteria;

3) proper model of biocolmation which implies the dependence of a change in porosity on the bacteria concentration. That is,

$$v = \frac{\left(1 - \varepsilon_0\right)\rho_m Q_s}{\rho_s \left(1 - f_\sigma\right)}, \quad \varepsilon = \varepsilon_0 - v,$$

where v is the total volume of bacteria growth; ε_0 is the initial porosity before filtration; ε is the porosity after filtration; Q_s is the volume fraction of clogged or precipitated material ($Q_s = AX$), A is the of sedimentation rate; ρ_m is the density of soil-sawdust material; ρ_s is the density of clogged or precipitated material; f_σ is the secondary porosity of precipitated material. The Kozani formula was used for the dependence of filtration factor on porosity.

Consequently, biocolmation as one of the consequences of microbial development leads to a change in hydrological parameters of the porous material of a geobarrier. However, in the known mathematical models of contamination propagation from waste storage facilities in the presence of a geobarrier, such changes were not taken into consideration. This is due to the difficulties of further exploration of such a mathematical model. Firstly, it requires modification of conjugation conditions for unknown functions. Secondly, this will require the use of effective numerical algorithms for solving a non-linear mathematical model. However, without the development of mathematical models in this direction, it is impossible to take into account a large number of field experiments and, consequently, to specify forecasts.

3. The aim and objectives of the study

The purpose of this study is to quantify the effect of the existence of microorganisms in soil pores on the value of head in a porous medium in general and, specifically, on the value of head drops during the transition through a thin geobarrier. This will make it possible to draw conclusions about the significant or insignificant changes in the predictive estimation of contamination propagation from waste storage facilities into groundwater.

To accomplish the aim, the following tasks have been set:

– to construct a mathematical model of the filtration of organic substances taking into consideration a biocolmation effect. Since the biocolmation effect causes a change in the hydrological parameters, in particular, a filtration factor, this phenomenon should be taken into consideration under conjugation conditions for heads;

– to find the numerical finite-element solutions to the corresponding non-linear boundary problem under the modified conjugation conditions, which describes the constructed mathematical model;

– to conduct a series of numerical experiments and perform their analysis.

4. Construction of a mathematical model of the filtration of organic substances taking into consideration the biocolmation effect

The article explored the process of the propagation of organic chemical substances in a soil layer of total thickness l with a thin inclusion of thickness d, which is placed at depth $x=\xi$ (Fig. 1).

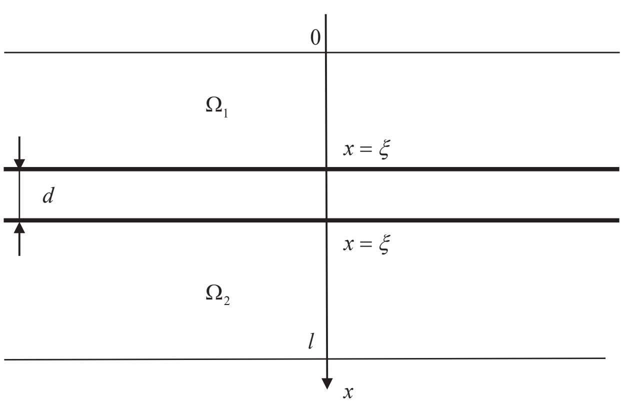

Fig. 1. Soil layer of thickness l with a thin inclusion of thickness d ($d \ll 1$)

To formulate the mathematical model, we will partially use the findings by scientists from the reviewing chapter of the article. The mathematical model will include the filtration equation under conditions of variable porosity. Its constituents should also be the equations of transfer of organic chemical substances in the pore fluid of the porous medium and the equation of the dynamics of bacteria biomass in the porous medium based on the Monod equation. As a result, we obtain the following boundary problem:

$$\beta\frac{\partial h}{\partial t}=\frac{\partial}{\partial x}\left(k(n)\frac{\partial h}{\partial x}\right),\quad x\in\Omega_1\cup\Omega_2,\quad t>0, \tag{1}$$

$$h(x,t)\big|_{x=0}=\bar{h}_0(t),\quad t\ge 0, \tag{2}$$

$$u(x,t)\big|_{x=l}=\left(-k(n)\frac{\partial h}{\partial x}\right)\bigg|_{x=l}=0,\quad t\ge 0, \tag{3}$$

$$h(x,0)=h_0(x),\quad x\in\bar{\Omega}_1\cup\bar{\Omega}_2, \tag{4}$$

$$n\frac{\partial c}{\partial t}=\frac{\partial}{\partial x}\left(nD\frac{\partial c}{\partial x}\right)-u\frac{\partial c}{\partial x}-\frac{\mu_{\max}}{Y}B\left(1-\frac{B}{B_{\max}}\right)\frac{c}{k_c+c},$$

$$x\in\Omega_1\cup\Omega_2,\quad t>0, \tag{5}$$

$$c(x,t)\big|_{x=0}=\bar{c}_0(t),\quad t\ge 0, \tag{6}$$

$$q_c(x,t)\big|_{x=l}=-nD\frac{\partial c}{\partial x}\bigg|_{x=l}=0,\quad t\ge 0, \tag{7}$$

$$c(x,0)=c_0(x),\quad x\in\bar{\Omega}_1\cup\bar{\Omega}_2, \tag{8}$$

$$\frac{\partial B}{\partial t}=\mu_{\max}B\left(1-\frac{B}{B_{\max}}\right)\frac{c}{k_c+c}-\mu_{dec}B,$$

$$x\in\Omega_1\cup\Omega_2,\quad t>0, \tag{9}$$

$$B(x,0)=B_0(x),\quad x\in\bar{\Omega}_1\cup\bar{\Omega}_2, \tag{10}$$

$$u^{\pm}\big|_{x=\xi}=-\frac{[h]}{\int_0^d\frac{dx}{k^{\gamma}(n^{\gamma})}}, \tag{11}$$

$$q_c^{\pm}\big|_{x=\xi}=-\frac{[c]}{\int_0^d\frac{dx}{n^{\gamma}D^{\gamma}}}. \tag{12}$$

Here:

– $\Omega_1=(0;\xi)$, $\Omega_2=(\xi;l)$, $0<\xi<l$, $\bar{h}_0(t)$, $h_0(x)$, $c_0(x)$, $\bar{c}_0(t)$, $B_0(x)$ are the known functions;

– β is the factor of the elastic capacity of soil;

– h is the head;

– k, k^{γ} are the factors of filtration of basic soil and inclusion soil, respectively;

– u is the filtration rate;

– n, n^{γ} are the porosity of soil and geobarrier material, respectively;

– q_c is the flow of chemical substances;

– μ_{dec} is the biomass decomposition factor;

– $u^{\pm}$, $q^{\pm}$ are the values of the rates of filtration and of the flows of chemical substances at $x=\xi-0$ and $x=\xi+0$, respectively;

– $[h]=h^{+}-h^{-}$, $[c]=c^{+}-c^{-}$ are the head drops and of concentration of organic chemical substances on thin inclusion;

– c is the concentration of the pore solution of the organic chemical substance;

– D is the factor of diffusion of an organic substance;

– $\mu_{\max}$ is the maximum rate of biomass growth;

– B is the concentration of bacteria biomass in the porous medium;

– $B_{\max}$ is the maximum possible concentration of bacteria biomass in the porous medium;

– k_c is the parameter in the equation of biomass dynamics, at which the rate of biomass growth is equal to half the maximum;

– Y is the bacterial yield.

Conjugation conditions (11), (12) differ from the classical ones and take into consideration the dependences of soil geobarrier parameters on porosity which, in turn, depend on the biomass concentration. Conditions (11), (12) are derived similarly to those from research [3].

5. Solving the problem on the filtration of organic substances taking into consideration the biocolmation effect in the area with inclusions by using a finite element method

Similarly to [19], let us assume that H_0 is the space of vector-functions $\{s_1(x); s_2(x); s_3(x)\}$, each component of which on each of the intervals $(0;\xi)$, $(\xi;l)$ belong to the Sobolev space $W_2^1(\Omega)$, in this case, the first two acquire zero values at the end of the segment $[0,l]$, where the boundary conditions of the first kind are assigned for functions $h(x,t)$ and $c(x,t)$, respectively. Let us assume that H is the space of functions $\{v_1(x,t); v_2(x,t); v_3(x,t)\}$, each component of which is integrated with the square along with its first variables $\partial v_i/\partial t$, $\partial v_i/\partial x$, $i=\overline{1,3}$ on each of intervals $(0;\xi)$, $(\xi;l)$, $\forall t\in(0;T]$, in this case, the first two satisfy the boundary conditions of the first kind like functions $h(x,t)$, $c(x,t)$, respectively. Here $T>0$.

Take $\{s_1(x); s_2(x); s_3(x)\}\in H_0$. Multiply equation (1) and initial condition (4) by $s_1(x)$, integrating them on the segment $[0, l]$ and taking into account conjugation conditions (11), obtain:

$$\int_0^l \beta\frac{\partial h}{\partial t}s_1(x)\mathrm{d}x + \int_0^l k(n)\frac{\partial h}{\partial x}\frac{\mathrm{d}s_1(x)}{\mathrm{d}x}\mathrm{d}x + \frac{[h][s_1]}{\int_0^d \frac{\mathrm{d}x}{k^\gamma(n^\gamma)}} = 0,\ \forall t\in(0;T], \tag{13}$$

$$\int_0^l h(x,0)s_1(x)\mathrm{d}x = \int_0^l h_0(x)s_1(x)\mathrm{d}x,\ \ \forall t\in(0;T]. \tag{14}$$

Similarly, for the concentration of organic chemical substances and biomass, we obtain:

$$\int_0^l n\frac{\partial c}{\partial t}s_2(x)\mathrm{d}x + \int_0^l nD\frac{\partial c}{\partial x}\frac{\mathrm{d}s_2(x)}{\mathrm{d}x}\mathrm{d}x + \int_0^l u\frac{\partial c}{\partial x}s_2(x)\mathrm{d}x + \frac{[c][s_2]}{\int_0^d\frac{\mathrm{d}x}{n^\gamma D}} + \int_0^l \frac{\mu_{\max}}{Y}\left(1-\frac{B}{B_{\max}}\right)B\frac{c}{k_c+c}s_2(x)\mathrm{d}x = 0,\ \forall t\in(0;T], \tag{15}$$

$$\int_0^l c(x,0)s_2(x)\mathrm{d}x = \int_0^l c_0(x)s_2(x)\mathrm{d}x,\ \ \forall t\in(0;T], \tag{16}$$

$$\int_0^l \frac{\partial B}{\partial t}s_3(x)\mathrm{d}x - \int_0^l \left(\mu_{\max}\left(1-\frac{B}{B_{\max}}\right)\times \frac{c}{k_c+c}-\mu_{dec}\right)Bs_3(x)\mathrm{d}x = 0,\ \forall t\in(0;T], \tag{17}$$

$$\int_0^l \mathrm{B}(x,0)s_3(x)\mathrm{d}x = \int_0^l B_0(x)s_3(x)\mathrm{d}x,\ \ \forall t\in(0;T]. \tag{18}$$

Attribute 1. Function $\{h(x,t); c(x,t); B(x,t)\}\in H$, which for any $\{s_1(x); s_2(x); s_3(x)\}\in H_0$ satisfies integral ratios (13)–(18), is called the generalized solution to the boundary problem (1) to (12).

We seek for the approximated solution to the boundary problem (1) to (12) in the form of:

$$h(x,t)=\sum_{i=1}^N h_i(t)\phi_{i1}(x),\quad c(x,t)=\sum_{i=1}^N c_i(t)\phi_{i2}(x),$$

$$B(x,t)=\sum_{i=1}^N B_i(t)\phi_{i3}(x), \tag{19}$$

where $h_i(t)$, $c_i(t)$, $B_i(t)$, $i=\overline{1,N}$, are the unknown factors that depend only on time. If we consider (19) as the approximated finite-element solution, functions $\phi_{i1}(x)$, $\phi_{i2}(x)$, $\phi_{i3}(x)$, $i=\overline{1,N}$, are the polynomial basis functions with a finite carrier. To simplify further calculations and in regard to numerical experiments, we will consider that the same grid of finite elements is used for approximated finding $h(x,t)$, $c(x,t)$ and $B(x,t)$. In this case, $\phi_{i1}(x)\equiv\phi_{i2}(x)\equiv\phi_{i3}(x)$ and to avoid double indexation, designate basic functions as $\phi_i(x)$, $i=\overline{1,N}$.

Then, from a weak statement (13) to (18) of problem (1) to (12), taking into account (19), we will obtain:

$$\mathbf{M}_1\cdot\frac{\mathrm{d}\mathbf{H}}{\mathrm{d}t}+\mathbf{L}_1(\mathbf{B})\cdot\mathbf{H}(t)=0, \tag{20}$$

$$\tilde{\mathbf{M}}_1\cdot\mathbf{H}^{(0)}=\tilde{\mathbf{F}}_1, \tag{21}$$

$$\mathbf{M}_2(\mathbf{B})\cdot\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t}+\mathbf{L}_2(\mathbf{H},\mathbf{B})\cdot\mathbf{C}(t)=0, \tag{22}$$

$$\tilde{\mathbf{M}}_2\cdot\mathbf{C}^{(0)}=\tilde{\mathbf{F}}_2, \tag{23}$$

$$\mathbf{M}_3\cdot\frac{\mathrm{d}\mathbf{B}}{\mathrm{d}t}+\mathbf{L}_3(\mathbf{C},\mathbf{B})\cdot\mathbf{B}(t)=0, \tag{24}$$

$$\tilde{\mathbf{M}}_3\cdot\mathbf{B}^{(0)}=\tilde{\mathbf{F}}_3, \tag{25}$$

where

$$\mathbf{H}=\left(h_i(t)\right)_{i=1}^N,\ \ \mathbf{C}=\left(c_i(t)\right)_{i=1}^N,\ \ \mathbf{B}=\left(b_i(t)\right)_{i=1}^N,$$

$$\mathbf{H}^{(0)}=\left(h_i(0)\right)_{i=1}^N,\ \ \mathbf{C}^{(0)}=\left(c_i(0)\right)_{i=1}^N,\ \ \mathbf{B}^{(0)}=\left(b_i(0)\right)_{i=1}^N,$$

$$\mathbf{M}_k=\left(m_{ij}^{(k)}\right)_{i,j=1}^N,\ \ \mathbf{L}_k=\left(l_{ij}^{(k)}\right)_{i,j=1}^N,\ \ \mathbf{F}_k=\left(f_i^{(k)}\right)_{i=1}^N,$$

$$\tilde{\mathbf{F}}_k=\left(\tilde{f}_i^{(k)}\right)_{i=1}^N,\ \ \tilde{\mathbf{M}}_k=\left(\tilde{m}_{ij}^{(k)}\right)_{i,j=1}^N,$$

$$\tilde{m}_{ij}^{(k)}=\int_0^l \phi_i\phi_j \mathrm{d}x,\quad k=\overline{1,3},$$

$$m_{ij}^{(1)}=\int_0^l \beta\phi_i\phi_j \mathrm{d}x,\quad \tilde{f}_i^{(1)}=\int_0^l h_0\phi_i \mathrm{d}x,$$

$$l_{ij}^{(1)}=\int_0^l k(n)\frac{\mathrm{d}\phi_i}{\mathrm{d}x}\frac{\mathrm{d}\phi_j}{\mathrm{d}x}\mathrm{d}x+\frac{[\phi_i][\phi_j]}{\int_0^d \frac{\mathrm{d}x}{k^\gamma(n^\gamma)}},$$

$$m_{ij}^{(2)}=\int_0^l n\phi_i\phi_j \mathrm{d}x,\quad \tilde{f}_i^{(2)}=\int_0^l c_0\phi_i \mathrm{d}x,$$

$$l_{ij}^{(2)}=\int_0^l nD\frac{\mathrm{d}\phi_j}{\mathrm{d}x}\frac{\mathrm{d}\phi_i}{\mathrm{d}x}\mathrm{d}x+\int_0^l u\frac{\mathrm{d}\phi_j}{\mathrm{d}x}\phi_i \mathrm{d}x+$$

$$+\int_0^l \frac{\mu_{\max}}{Y}\left(1-\frac{B}{B_{\max}}\right)\frac{B}{k_c+c}\phi_j\phi_i \mathrm{d}x+\frac{[\phi_i][\phi_j]}{\int_0^d \frac{\mathrm{d}x}{n^\gamma D}},$$

$$m_{ij}^{(3)}=\int_0^l \phi_i\phi_j \mathrm{d}x,\quad \tilde{f}_i^{(3)}=\int_0^l B_0\phi_i \mathrm{d}x,$$

$$l_{ij}^{(3)}=-\int_0^l\left(\mu_{\max}\left(1-\frac{B}{B_{\max}}\right)\frac{c}{k_c+c}-\mu_{dec}\right)\phi_j\phi_i \mathrm{d}x.$$

The system of equations (20) to (25) is the Cauchy problem for a system of non-linear differential first-order equations. Finding its solution also requires the use of appropriate discretization schemes.

6. Schematic algorithm of the finite-element solution to problem (1) to (12) and time sampling

Step 0. The actions of this step are based on the ideas from [19]. Cover $[0;\xi]\cup[\xi;l]$ with a finite-element grid. In this case, there are such two finite elements $[x_{m-1};x_m]\in[0;\xi]$ and $[x_{m+1};x_{m+2}]\in[\xi;l]$ that $x_m=x_{m+1}=\xi$ and $x_m\in[0;\xi]$, $x_{m+1}\in[\xi;l]$. The basis functions $\phi_m(x)$ and $\phi_{m+1}(x)$ are discontinuous at $x=\xi$, that is:

$$\phi_m(x)\big|_{x=\xi-0}=1,\ \phi_m(x)\big|_{x=\xi+0}=0,$$

$$\phi_{m+1}(x)\big|_{x=\xi-0}=0,\ \phi_{m+1}(x)\big|_{x=\xi+0}=1.$$

Step 1. Find $\mathbf{H}^{(0)}$, $\mathbf{C}^{(0)}$ and $\mathbf{B}^{(0)}$. In practice, to perform this step of the system of linear algebraic equations (SLAE), (21), (23) are (25) not to be solved. Taking into consideration the properties of basic functions of the method of finite elements ($\phi_i(x_i)=1,\ i=\overline{1,N}$), we find the values of factors $h_i(t)$, $c_i(t)$, $b_i(t)$, $i=\overline{1,N}$ at the initial moment of time $t=0$ directly from initial conditions (4), (8), (10):

$$h_i(0)=h_0(x_i),\quad c_i(0)=c_0(x_i),$$

$$b_i(0)=B_0(x_i),\quad i=\overline{1,N}.$$

Assign value 0 to index p. For simplification, time sampling will be performed on a uniform grid at pitch τ. Assign the number of pitches M in time.

Step 2. To find $\mathbf{H}^{(p+1)}$, perform discretization of the system of non-linear differential equations (20) in time with the use of completely implicit linearized differential scheme [6]:

$$\mathbf{M}_1\cdot\frac{\mathbf{H}^{(p+1)}-\mathbf{H}^{(p)}}{\tau}+\mathbf{L}_1\left(\mathbf{B}^{(p)}\right)\cdot\mathbf{H}^{(p+1)}=0,\quad p=1,2,\ldots$$

where $\mathbf{H}^{(p)}=\mathbf{H}(t_p)$, $\mathbf{B}^{(p)}=\mathbf{B}(t_p)$, $t_p=p\tau$.

After the formation of the SLAE:

$$\mathbf{G}\cdot\mathbf{H}^{(p+1)}=\mathbf{F},$$

where

$$\mathbf{G}=\frac{1}{\tau}\mathbf{M}_1+\mathbf{L}_1(\mathbf{B}^{(p)}),$$

$$\mathbf{F}=\frac{1}{\tau}\mathbf{M}_1\cdot\mathbf{H}^{(p)},$$

the main boundary condition – the boundary condition of the first kind (2) – must be taken into consideration. It is considered by the implementation of the two following steps:

1) all the elements of the first SLAE equation, including a free term, are zeroed;

2) the first element of the first equation is equal to 1, and a free term is taken equal to $\bar{h}_0(t_{p+1})$.

To find the integrals during the formation of **G** and **F,** we use numerical integration.

Step 3. Similarly**,** we find $\mathbf{C}^{(p+1)}$ from (22) and $\mathbf{B}^{(p+1)}$ from (24).

Step 4. Increase p by 1. If $(p+1)>M$, complete calculation. Otherwise, proceed to step 2.

7. The results of numerical experiments on solving the problem of the filtration of organic substances taking into consideration the biocolmation effect

Parameters of soils for numerical experiments were taken from the freely available software Hydrus-1D. In particular, Silt Loam at $k_0=0.108$ m/day, $n_0=0.45$, where index «0» means initial values, was considered as the basic soil. The clay with the following parameters $k_0^\gamma=0.0048$ m/day, $n_0^\gamma=0.36$ was used as the thin inclusion soil:

The soil layer of thickness $l=10$ m was considered for a model problem. The depth of the inclusion deposit was $\xi=2$ m, and its thickness $d=0.2$ m. The pitch of variable x was 0.02 m. The time pitch $\tau=1$ day.

The equation of filtration consolidation [20], where $\beta=\gamma_c a/(1+e)$, $e=n/(1-n)$ is the soil porosity factor, $a=5.12\cdot10^{-5}$ m^2/H is the soil compactness factor, $\gamma_c=10^4$ H/m^3 is the specific weight of pore solution, was considered as equation (1). The initial distribution of heads $h_0(x)=10$ m, which corresponds to the application to soil of the corresponding load – wastes that are the source of the organic substances. The free fluid outflow is ensured at the lower boundary, while there is no drain at the upper boundary.

Glucose solution was considered as an organic solution. The initial glucose distribution in pore water $c_0(x)=1$ mM. In boundary condition (6) on the soil surface $\bar{c}_0(t)=10$ mM. The factor of glucose diffusion is $D=0.5184\cdot10^{-4}$ m^2/day.

Dependence [12] was used for the dependence of filtration factor on porosity:

$$\frac{k}{k_0}=\left(\frac{n_0-n_B}{n_0}\right)^{19/6},$$

where n_B is the biomass volume in the unit of volume of the porous medium. To convert the biomass concentration to volume, use the assumption that 80 % of biovolume is water, the remaining 20 % is dry mass – 50 % carbon (bio-carbon) [21]. That is,

$$n_B=\frac{B}{0.8\rho_w+0.2\cdot(\rho_c/2)},$$

where ρ_w is the density of water; ρ_c is the density of bio-carbon. The complexity is that, for example, for bacteria colonies, value ρ_c varies in the range from 50 to 650 kg/m^3 [17]. In numerical experiments $\rho_c=100\,\text{kg/m}^3$ parameters of biomass kinetics are the following: $\mu_{\max}=0.2\,\text{day}^{-1}$, $B_{\max}=100\,\text{kg/m}^3$, $\mu_{dec}=0.01\,\text{day}^{-1}$, $k_c=0.06\,\text{mM}$, $Y=50$.

Piecewise-quadratic functions were used on the basis functions of the MFE. The results of numerical experiments are given in Tables 1, 2.

Table 1

Values of heads and their drops on the inclusion when biocolmation is neglected

Moment of time	h^-	h^+	$[h]$
t=25 days	9.639	8.936	0.703
t=50 days	8.390	7.090	1.300
t=100 days	5.689	4.550	1.139
t=200 days	2.431	1.925	0.506
t=300 days	1.032	0.817	0.215

Table 2

Values of heads and their drops on the inclusion when biocolmation is taken into consideration

Moment of time	h^-	h^+	$[h]$
t=25 days	9.770	9.157	0.613 (–12.8 %)
t=50 days	9.100	7.515	1.585 (+21.9 %)
t=100 days	6.919	5.156	1.763 (+54.8 %)
t=200 days	3.214	2.445	0.769 (+52.0 %)
t=300 days	1.404	1.093	0.311 (+44.6 %)

Table 2 corresponds to the use of the modified conjugation conditions, and the results of Table 1 – to the classic ones [19]. Table 2 shows a relative increase (as a percentage with a «plus» sign) or a relative decrease (with a «minus» sign) in the values of head drops on a thin inclusion in comparison with the case when the biocolmation influence is neglected (the values in Table 1).

8. Discussion of results of solving the problem on the filtration of organic substances taking into consideration the biocolmation effect

As the comparison of data from Table 1 and Table 2 reveals, considering a dynamic change in the microorganisms in the porous medium affects the value of heads from the bottom and from the top of a protective geobarrier. And while the values of heads at the top (h^-) are determined by the existence of microorganisms in the soil before a geobarrier, the values at the bottom (h^+) are determined by the development of microorganisms in the thin inclusion itself and the use of modified conjugation conditions (Table 2). These changes are clearly traced through the values of drops $[h]$: in the presence of microorganisms, excessive heads, as a consequence of the applied external loads from wastes, propagate more slowly in the vicinity of a geobarrier. In this case, due to the nonlinearity of the influences and complex interdependences of processes, it is impossible to predict such values and their differences without computer simulation and mathematical modeling. In practice, our research can be used to assess the propagation of organic contamination from waste storage facilities, because their dynamics depends on the head gradient (drop) in a geobarrier. In addition, since clays are the material for artificial geobarriers, the changes in heads in the neighborhood of a thin inclusion (especially, an increase in drops, which means an increase in the gradient of a drop) can lead to the formation of landslide hazardous zones, which is especially important for large waste storage facilities. Such clarification in the estimation calculations can be considered in the preparation of design documentation and engineering features of organic waste storage facilities. However, the hydrological characteristics of soils and the parameters of the dynamics of microorganisms' growth should be known to make such calculations possible. The problem of the relationships between biomass and biological volume of microorganisms is far from trivial. It imposes some constraints on the research results. This study will be developed in the following way:

1) the consideration of design features of waste storage facilities and the arrangement of a geobarrier, which is possible by increasing the dimensionality of the problem;

2) taking into account the models of the dynamics of microorganisms based on the differential equations in the partial second-order derivatives;

3) theoretical study into the accuracy of the derived finite element solutions for boundary problems with the modified conjugation conditions.

9. Conclusions

1. A mathematical model of the filtration of organic substances in the soil array in the presence of a thin geobarrier was constructed taking into consideration the biocolmation effect, which includes the filtration equation under conditions of variable porosity. Since the hydrological parameters of the materials of geobarriers depend greatly on the activity of microorganisms, the model uses the idea of modifying the conjugation conditions for heads, taking into consideration these effects. In addition, the components of the model are the equation of the transfer of organic chemical substances in the pore fluid of the porous medium and the equation of the dynamics of bacteria biomass in a porous medium based on the Monod equation.

2. Numerical solutions to the corresponding nonlinear boundary problem were derived by using the method of finite elements (MFE). The schematic algorithm of the finite-element solution to the obtained problem, including the scheme of time sampling, is presented. The application of the MFE to the problems of this type is substantiated by the necessity of finding generalized solutions, in which discontinuities of the first kind are possible. Based on the developed algorithms, a software suite for carrying out numerical experiments has been developed, which implies taking into account the modified conjugation conditions.

3. Computer simulation has revealed that the presence of microorganisms in the pores of soil significantly affects the values of heads at the top and at the bottom of a geobarrier, hence, the values of head drops. In particular, the biocolmation of a geobarrier (based on the solution to a model problem) can lead to a relative increase in a head drop by 54.8 % compared to the case of disregarding the activity of microorganisms. Such differences, in turn, lead to changes in the predictive calculations of contamination propagation from waste storage facilities into groundwater and can cause negative changes in the stressed-strained state of the soil array in the geobarrier neighborhood as a thin inclusion. At the same time, due to the nonlinearity of influences and complex interdependence of the processes, it is impossible to predict such values and their differences without computer simulation and mathematical modeling. In addition, the hydrological characteristics of soils and the parameters of the dynamics of microorganism growth should be known.

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APPLYING A MODIFIED ALUMINUM SULFATE SOLUTION IN THE PROCESSES OF DRINKING WATER PREPARATION

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This paper reports a study on the application of aluminum sulfate solution, modified by the magnetic field and electrocoagulation, in the processes of drinking water preparation. The modification of the coagulant solution makes it possible to intensify water purification processes, to reduce reagent consumption by 25–30 %. It has been found that a dose of the modified aluminum sulfate solution of 28–30 mg/dm³ improves the efficiency of removal of suspended substances and coloration by 35–40 %. The dosage of the conventional reagent solution was 40 mg/dm³ while reaching the same purification parameters.

Modifying a solution of aluminum sulfate with the magnetic field and electrocoagulation increases the hydraulic size of the coagulated suspension. A change in the hydraulic size in the suspension has been studied at different periods of the year. In winter, when treating water with the modified aluminum sulfate solution, there a decrease in the suspension content whose hydraulic size is 0.1 mm/s and less, from 89 % to 22 %. In this case, the content of suspended substances at settling decreases from 8.5–12.5 mg/dm³ to 5.6–8.3 mg/dm³. In spring, when using the modified coagulant solution, the content of suspension whose size is 0.1 mm/s and less decreased from 55 % to 15 %. In summer, there is an increase in the content of suspension whose size is 0.3–0.5 mm, from 58 % (a conventional reagent solution) to 66 % (the modified reagent solution). This indicates an intensification of the coagulation of impurities and the clarification of water.

The experimental data testify to an increase in the effectiveness of discoloration of natural low-turbid colored water to 63.3–63.9 % for the modified reagent solution at 45.5 % for a conventional reagent solution.

A change in the bacteriological parameters has been determined: the effectiveness of the decrease in a microbial number grows from 11.6–18.7 % to 18.6–25.1 %. In terms of a coli-index, the efficiency of purification grows from 16.6–23.1 % to 23.0–29.5 %

Keywords: drinking water quality, modification of reagent solution, coagulation, aluminum sulfate, hydraulic size, coloration, suspended substances, water clarification, magnetic field, anode-dissolved iron

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1. Introduction

The purification of water from the surface sources of water supply, used to provide drinking needs, from coarsely-dispersed, colloidal, and other contaminants, mostly employs the physical-chemical technology. This technology includes the processes of settling and filtration, which are important elements of water supply systems in the preparation of drinking water [1, 2].

One of the most common methods of water purification from coarsely-dispersed and colloidal contaminants is the method of water treatment by coagulants. However, under