NUMERICAL SIMULATION OF THE EFFECT OF CHEMICAL OSMOSIS ON THE VALUE OF THE JUMPS OF POLLUTION IN THE GEOCHEMICAL BARRIER

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Abstract: The mathematical model of the propagation of chemical substances in the soil that contains a thin clay geobarrier was investigated. The function of the geobarrier as an integral element of the soil base of waste storage facilities is the limitation of the spread of harmful substances outside the facility. The developed mathematical model takes into account: 1) the ideality properties of the barrier material; 2) the phenomenon of chemical osmosis; 3) the conjugation conditions account for the dependence of the filtration coefficient, the degree of ideality, the diffusion coefficient on the concentration of the chemicals. The necessity to consider such dependencies is substantiated by the review of scientific publications with the corresponding data of field experiments. The numerical solution of the corresponding non-linear boundary value problem was found by the finite element method. The numerical experiments show the significance of considering chemical osmosis in the prediction calculations of the spread of harmful chemicals through geobarriers.

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1. Introduction

When liquid inorganic chemical contaminants enter into clay soil, osmotic phe-

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nomena may appear in the porous medium. This is due to the specific properties of clay soils and the possibility of their action as semi-permeable membranes. These are membranes that have a rather high permeability not for all but only for some substances, in particular for solvents. Osmosis is a one-sided diffusion through a semi-permeable membrane that separates the solution from a pure solvent or a solution of lower concentration. This phenomenon is explained by the gravitation of the system to thermodynamic equilibrium and the leveling of the concentration of the solutions on both sides of the membrane. It is characterized by osmotic pressure that is equal to the excessive external pressure which must be applied from the side of the solution to stop osmosis [10, 19]. A detailed analysis (164 primary sources) of the research of osmotic effects in porous media including both theoretical and experimental developments was performed in [17]. The problems and effects of chemical osmosis, electro-osmosis and thermal osmosis were revealed. As noted in [5], it is the soils with low permeability, which include clay, that can operate as semi-permeable membranes that generate osmotic flow.

Although much investigation of osmosis for clay soils has been performed, both in terms of on-site experimental research and predictive mathematical modeling [28, 29], some aspects have not been taken into account so far. One of these is osmotic phenomena under the conjugation conditions for thin geosynthetic barriers in the soil base of the storage facilities for household and industrial wastes. As practice shows, clay and geosynthetic barriers are widely used in the construction of such facilities. A detailed review (a total of 128 primary sources) of the reports on the use of geosynthetic thin coatings (inclusions) in waste storage facilities was performed in [9]. The authors note that such inclusions of geosynthetic clay materials began to be widely used since 1970s. Their primary function is to restrict the spread of harmful substances from waste storage facilities to the environment. The use of artificial geosynthetic bentonite geobarriers in the waste storages was reviewed in [22]. It is noted that industrial GCL (geosynthetic clay liners) are currently manufactured as panels of 4.2–5.3 meter width, 30–61 meter length, and 15 to 30 mm thickness. According to scientific sources, GCLs as finished panels were used for the first time in 1986.

A review of current technologies and research on the use of improved bentonites as geobarriers for inorganic waste storage was the objective of [23]. They focused on three characteristics: the filtration coefficient, the effective diffusion coefficient and the membrane ideality coefficient ω (the chemico-osmotic efficiency coefficient of the membrane). The necessity to improve the properties of the geosynthetic bentonite geobarriers arises from certain solutions of chemical

industry waste to which bentonites are still not stable and are weak as function-
ing protective and restraining barriers. Processes of mechanical and chemical
consolidation of clay materials that exhibit the properties of semipermeable
membranes are investigated in [30]. They used a modification of the Darcy law

$$v_u + v_\pi = -k\frac{\partial h}{\partial z} + \omega\frac{k}{\gamma}\frac{\partial \pi}{\partial z} = -k\frac{\partial h}{\partial z} + \omega\frac{RT}{M}\frac{k}{\gamma}\frac{\partial c}{\partial z},$$

where ω is the chemico-osmotic efficiency coefficient of the membrane; M is
the molar mass of the solute; k is the filtration coefficient; π is the osmotic
pressure; R is the universal gas constant; T is the absolute temperature; c is
the concentration of chemicals in the pore fluid. It was also noted that according
to [7]

$$k = k_0\left(\frac{n}{n_0}\right)^3,$$

where n is porosity; k_0, n_0 are the initial values of the filtration coefficient
and of porosity. It should be noted that the issues of chemical and thermal
consolidation of soils taking into account osmotic phenomena were also studied
in [28, 29]. However, the heterogeneity of the environment and the presence of
thin semipermeable inclusions were not considered. For a flow of a chemical
solution we have

$$q_c = (1 - \omega)v_u c + v_\pi c - nD^*\frac{\partial c}{\partial z},$$

where D^* is the effective diffusion coefficient including "the tortuosity of porous
media flow paths". It was shown in [13] for semipermeable clay materials that

$$D^* = \tau(1 - \omega)D_0,$$

where D_0 is the diffusion coefficient for a solution in the porous liquid; τ is the
tortuosity factor and $0 < \tau < 1$. According to [12]

$$\tau = n^m,$$

where m is an empirical parameter. Also, numerical experiments were per-
formed and certain numerical parameters of the model were determined in [30].

   Chemical osmosis in [19] is defined as the possibility of the movement of
water (solvent) under the influence of salt concentration difference. In this case,
the generalized Darcy law takes the form

$$q = -k\frac{\partial h}{\partial x} + \omega k\frac{\partial \pi_h}{\partial x}.$$

Here k is the filtration coefficient; h is the heads; π_h is the osmotic heads, or $\pi_h = \frac{\pi}{\rho g} = \frac{\pi}{\gamma}$, where π is the osmotic pressure. Osmotic pressure is defined as [3]

$$\pi = \frac{RT}{v_w} \ln(a_w),$$

where R is the universal gas constant; T is the temperature; v_w is the molar volume of water; a_w is water activity (dimensionless value).

It was experimentally established in [24] that the effective diffusion coefficient of KCl solution in geosynthetic bentonite geobarriers non-linearly depends on the value of the input concentration C_0 (Table 1). The dependence of the ideality coefficient on C_0 is also presented. Obtained experimental results confirm the possibility of significant mutual effect of the concentration of chemical substances dissolved in pore water and physico-chemical parameters of the porous medium.

$C_0(mM)$	$D \times 10^{-5} \left(m^2/day\right)$	ω
20	0.76896	0.37
35	0.93312	0.24
50	1.01088	0.18
100	1.08864	0.11
200	1.08864	0.11
400	1.22688	0

Table 1. Dependence of the effective diffusion coefficient and the ideality coefficient of geosynthetic geobarrier on the input concentration of KCl [24]

The ratio of the filtration coefficient k_0 of the geosynthetic barrier in the presence of KCl solution of concentration C_0 in the pores to the filtration coefficient K_0 in pure water was investigated in [14]. The results shown in Table 2 testify to the need to take into account even modest concentrations of chemical solutions in pores through the change in filtration characteristics of geobarriers. After all, the filtration coefficient k_0 increases 1.65 times faster than K_0 with increasing KCl concentration to $C_0 = 50mM$.

$C_0\ (mM)$	k_0/K_0
0	1
10	1.2
20	1.35
30	1.5
40	1.6
50	1.65

Table 2. Dependence of the filtration coefficient ratio of geosynthetic geobarrier on the input concentration of KCl [14]

The above research overview outlines existing developments and still outstanding tasks regarding the spread of pollutants in environments with clay geobarriers. Particularly, the well-known modifications of the Darcy law can take into account the ideality properties (coefficient ω) as well as the phenomena of osmosis for geobarriers. The results of many reports point to the importance of such tasks in terms of ecology and environmental protection. However, the results of field experiments show that the filtration coefficient k and the ideality coefficient ω non-linearly depend both on the concentration of chemicals c and the humidity θ. Therefore, the corresponding mathematical model of the distribution of pollutants in an unsaturated medium with thin clay inclusions will be described by a boundary value problem with non-linear dependence of coefficients on unknown functions. Moreover, in [6] the conjugation conditions were modified for the presence of osmosis phenomena and for non-linear dependence of the parameters of thin inclusions on the determinant functions of processes (concentration of chemical solutions and humidity). However, no studies of the effect of such dependences on the processes themselves were performed. That is the objective of this article.

The process of the spread of dissolved substances by diffusion through a soil mass acting as a limiting geobarrier for the contaminants was considered in [4]. Assuming linear pressure distribution in the pore fluid, the generally non-linear diffusion equation was reduced to a linear one. Due to this, an analytical solution to the respective boundary value problem was found. Generally, numerical methods have to be applied in the case of non-linear problems. The investigation of the effect of the non-linear dependences $k = k(c, \theta)$ and $\omega = \omega(c)$ as well as the osmosis phenomenon itself on the spread of pollutants in the environment with geobarriers requires solving a non-linear boundary value problem for the systems of differential equations of parabolic type. The complexity of the problem is determined also by the possibility of occurrence of discontinuities in solutions.

The application of the finite element method (FEM) to models of hydraulic fracturing of the formation in a porous medium is described in [15]. The gap and the jump in the fields of the head is "smoothed out" (reduces to a continuous case) through the introduction of the concept of "weak rupture". Algorithmic and computational aspects of the application of FEM to mathematical models of hydraulic fracturing in porous media with possible discontinuities in the solutions are discussed in [20]. Discretization of the two-dimensional problem utilized finite elements of two types, classic triangular finite elements in the

sub-regions without cracks, and finite elements of zero "thickness" with triple
nodes in the split itself (one node on one side of the crack, another in the
center of the crack that belongs to a one-dimensional finite element, the third
one on the other side of the crack). In the assumption of small deformations,
the thickness of the crack during the discretization is disregarded. The idea of
triple nodes is the expansion of the idea of dual nodes in the places of possible
discontinuities in the solution [25, 26].

A new approach (according to the authors) to the numerical study of the
process of the propagation of cracks in heterogeneous media which may con-
sist of discrete elements is proposed in [2]. Among the numerical methods,
the attention is focused on FEM, an overview of its existing modifications and
development of new ones. Thus, the scientists consider FEM one of the key
methods for finding approximate solutions of boundary value problems in het-
erogeneous media with inclusions. This is due to the possibility of finding the
most generalized approximate solutions. Given the relative simplicity of imple-
mentation, in this paper we use the approach to numerical solution of this type
of problems that is described in [25, 26].

2. A mathematical model of the problem

Consider a one-dimensional case. The interconnected process of the variation
of the heads and the concentration of a chemical substance in a pore solution
of an unsaturated heterogeneous soil mass in the presence of chemical osmosis
is described by the following boundary-value problem:

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

$$h(x,t)|_{x=0} = \overline{h}_0(t), t \geq 0; \tag{2}$$

$$u(x,t)|_{x=l} = \left(-k(h,c)\frac{\partial h}{\partial x} + k(h,c) - k_c(h,c)\frac{\partial c}{\partial x}\right)\Bigg|_{x=l} = 0, t \geq 0; \tag{3}$$

$$h(x,0) = h_0(x), x \in [0;\xi] \cup [\xi;l]; \tag{4}$$

$$\theta(h)\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(\theta(h)D(h,c)\frac{\partial c}{\partial x}\right) - u\frac{\partial c}{\partial x}, x \in \Omega_1 \cup \Omega_2, t > 0; \tag{5}$$

$$c(x,t)|_{x=0} = \overline{c}_0(t), t \geq 0; \tag{6}$$

$$q_c(x,t)|_{x=l} = -\theta(h)D(h,c)\frac{\partial c}{\partial x}\bigg|_{x=l} = 0, t \geq 0; \tag{7}$$

$$c(x,0) = c_0(x), x \in [0;\xi] \cup [\xi;l]; \tag{8}$$

$$u^{\pm}|_{x=\xi} = -\frac{[h]}{\int_0^d \frac{dx}{k^\gamma(h,c)}} + \frac{d}{\int_0^d \frac{dx}{k^\gamma(h,c)}} + \frac{1}{\int_0^d \frac{dx}{k^\gamma(h,c)}}\int_0^d \frac{k_c^\gamma(h,c)}{k^\gamma(h,c)}\frac{\partial c}{\partial x}dx; \tag{9}$$

$$q_c^{\pm}|_{x=\xi} = -(1-\omega(\theta,c))\frac{[c]}{\int_0^d \frac{dx}{\theta(h)D^\gamma(h,c)}}. \tag{10}$$

Eqs. (1), (5) neglect the internal sources and drains of moisture and chemicals including mass transfer processes. Here d is the thickness of the thin inclusion; $\Omega_1 = (0;\xi)$, $\Omega_2 = (\xi;l)$, $0 < \xi < l$; $\overline{c}_0(t)$, $\overline{h}_0(t)$, $c_0(x)$, $h_0(x)$ are known functions; k_c and k_c^γ are the osmosis coefficients of the main soil and the fine inclusion, respectively, with $k_c = \omega(h,c)\frac{RT}{M}\frac{k(h,c)}{\gamma}$, $k_c^\gamma = \omega^\gamma(h,c)\frac{RT}{M}\frac{k^\gamma(h,c)}{\gamma}$, and $\omega(h,c)$, $\omega^\gamma(h,c)$ are the chemico-osmotic efficiency coefficients of the membrane. Functions $h_0(x)$, $c_0(x)$ must be continuous at each of the segments $[0;\xi]$, $[\xi;l]$. Eq. (1) is the moisture transfer equation [1, 27]. According to van Genuchten's model [27],

$$\theta(h) = \theta_{\min} + \frac{\theta_{\max} - \theta_{\min}}{(1+(-\alpha h)^n)^m}, k(h) = k_0\sqrt{s}(1-(1-s^{\frac{1}{m}})^m)^2,$$

where $\theta \in [\theta_{\min};\theta_{\max}]$, $\theta_{\min} > 0$, $\theta_{\max} \in (\theta_{\min};1]$, $n > 1$, $m = 1 - \frac{1}{n}$; $s = \frac{\theta-\theta_{\min}}{\theta_{\max}-\theta_{\min}}$ is relative humidity; k_0 is the filtration coefficient (for full saturation with $s = 1$ and $h = 0$). Further,

$$\beta(h) = \frac{d\theta}{dh} = \alpha nm(\theta_{\max} - \theta_{\min})(1+(-\alpha h)^n)^{-m-1}(-\alpha h)^{n-1}.$$

Also, the filtration coefficient k_0 significantly depends on the concentration of chemicals dissolved in the pore fluid [11, 14].

Conditions (9), (10) are the modified conjugation conditions in the case of the dependence of the parameters of fine inclusion and its ideality degree on physico-chemical factors as well as the consideration of chemical osmosis [6]. Here q_c is the flow of chemicals through the fine inclusion; $[c] = c^+ - c^-$ is the value of the gap in the concentration of chemicals at the inclusion. Since we place the source of moisture and chemical contaminants on top ($x = 0$), then the ideality coefficient is assumed to depend on the concentration of chemicals and the humidity at $x = \xi - 0$.

3. Solving the problem in the area with the inclusion by the finite element method

Similarly to [25, 26], we introduce a number of definitions and spaces. Let H_0 be a space of vector-valued functions $\{s_1(x);\ s_2(x)\}$ each of the components of which at each of the intervals $(0;\xi)$, $(\xi;l)$ belong to the Sobolev space $W_2^1(\Omega)$ and acquire zero values at the ends of the segment $[0, l]$ where the boundary conditions of the first kind are set for the functions $h(x, t)$, $c(x, t)$, respectively. Let H be a space of functions $\{v_1(x, t);\ v_2(x, t)\}$ each component of which is square-integrable along with the first derivatives $\frac{\partial v_i}{\partial t}$, $\frac{\partial v_i}{\partial x}$, $i = 1, 2$ at each of the intervals $(0;\xi)$, $(\xi;l)$, $\forall t \in (0;T]$, and satisfy the same boundary conditions of the first kind as the functions $h(x, t)$, $c(x, t)$, respectively. Here $T > 0$.

Let $\{s_1(x);\ s_2(x)\} \in H_0$. Multiplying Eq. (1) and the initial condition (4) by $s_1(x)$, integrating them over the segment $[0, l]$ and taking into account the conjugation condition (9), we obtain

$$
\int_0^l \beta(h)\frac{\partial h}{\partial t}s_1(x)dx + \int_0^l k(h, c)\frac{\partial h}{\partial x}\frac{ds_1(x)}{dx}dx + \frac{[h]\,[s_1]}{\int_0^d \frac{dx}{k^\gamma(h,c)}}
$$

$$
- \int_0^l k_c(h, c)\frac{\partial c}{\partial x}\frac{ds_1(x)}{dx}dx - \frac{[c]\,[s_1]}{d}\frac{\int_0^d \frac{k_c^\gamma(h,c)}{k^\gamma(h,c)}dx}{\int_0^d \frac{dx}{k^\gamma(h,c)}}
$$

$$
= \int_0^l k(h, c)\frac{ds_1(x)}{dx}dx + \frac{d\,[s_1]}{\int_0^d \frac{dx}{k^\gamma(h,c)}}, \forall t \in (0;T]; \tag{11}
$$

$$
\int_0^l h(x, 0)s_1(x)dx = \int_0^l h_0(x)s_1(x)dx, \forall t \in (0;T]. \tag{12}
$$

Similarly, from Eqs. (5) and (8)

$$
\int_0^l \theta(h)\frac{\partial c}{\partial t}s_2(x)dx + \int_0^l \theta(h)D(h, c)\frac{\partial c}{\partial x}\frac{ds_2(x)}{dx}dx + \int_0^l u\frac{\partial c}{\partial x}s_2(x)dx
$$

$$+ (1 - \omega(\theta^-, c^-)) \frac{[c]\,[s_2]}{\int\limits_0^d \frac{dx}{\theta(h)D^\gamma(h,c)}} = 0, \quad \forall t \in (0; T]; \tag{13}$$

$$\int\limits_0^l c(x, 0) s_2(x) dx = \int\limits_0^l c_0(x) s_2(x) dx, \forall t \in (0; T]. \tag{14}$$

Definition 1. A function $\{h(x,t); c(x,t)\} \in H$ which for any $\{s_1(x); s_2(x)\} \in H_0$ satisfies the integral relations (11)–(14) is called a generalized solution of the boundary value problem (1)–(10).

An approximate generalized solution of the boundary value problem (1)–(10) is sought in the form

$$h(x, t) = \sum_{i=1}^N a_i(t)\phi_{i1}(x), c(x, t) = \sum_{i=1}^N b_i(t)\phi_{i2}(x), \tag{15}$$

where $\{\phi_{i1}(x); \phi_{i2}(x)\}$, $i = \overline{2, N}$ are basis vector-functions of finite-dimensional subspace $M_0 \in H_0$ and functions $\phi_{11}(x)$, $\phi_{12}(x)$ are used for the approximation of non-uniform boundary conditions of the first kind (2) and (6).

Further, from the weak formulation (11)–(14) of the problem (1)–(10), taking into account (15), we obtain the Cauchy problem

$$\mathbf{M}_{11}(\mathbf{A}, \mathbf{B}) \cdot \frac{d\mathbf{A}}{dt} + \mathbf{L}_{11}(\mathbf{A}, \mathbf{B}) \cdot \mathbf{A}(t) + \mathbf{L}_{12}(\mathbf{A}, \mathbf{B}) \cdot \mathbf{B}(t) = \mathbf{F}_{11}(\mathbf{A}, \mathbf{B}), \tag{16}$$

$$\tilde{\mathbf{M}}_1 \cdot \mathbf{A}^{(0)} = \tilde{\mathbf{F}}_1, \tag{17}$$

$$\mathbf{M}_{22}(\mathbf{A}, \mathbf{B}) \cdot \frac{d\mathbf{B}}{dt} + \mathbf{L}_{22}(\mathbf{A}, \mathbf{B}) \cdot \mathbf{B}(t) = \mathbf{F}_{22}(\mathbf{A}, \mathbf{B}), \tag{18}$$

$$\tilde{\mathbf{M}}_2 \cdot \mathbf{B}^{(0)} = \tilde{\mathbf{F}}_2, \tag{19}$$

where $\mathbf{A} = (a_i(t))_{i=1}^N, \mathbf{A}^{(0)} = (a_i(0))_{i=1}^N, \mathbf{M}_{kk} = (m_{ij}^{(kk)})_{i,j=1}^N, \mathbf{L}_{kk} = (l_{ij}^{(kk)})_{i,j=1}^N,$
$\mathbf{F}_{kk} = (f_i^{(kk)})_{i=1}^N, \tilde{\mathbf{F}}_k = (\tilde{f}_i^{(k)})_{i=1}^N, \tilde{\mathbf{M}}_k = (\tilde{m}_{ij}^{(k)})_{i,j=1}^N, k = 1, 2, \mathbf{L}_{12} = (l_{ij}^{(12)})_{i,j=1}^N;$

$$m_{ij}^{(11)} = \int\limits_0^l \beta(\hat{h})\phi_{i1}\phi_{j1}dx, \tilde{m}_{ij}^{(1)} = \int\limits_0^l \phi_{i1}\phi_{j1}dx, \tilde{f}_i^{(1)} = \int\limits_0^l h_0\phi_{i1}dx,$$

$$l_{ij}^{(11)} = \int\limits_0^l k(\hat{h}, \hat{c})\frac{d\phi_{i1}}{dx}\frac{d\phi_{j1}}{dx}dx + \frac{[\phi_{i1}]\left[\phi_{j1}\right]}{\int\limits_0^d \frac{dx}{k^\gamma(\hat{h},\hat{c})}},$$

$$l_{ij}^{(12)} = \frac{[\phi_{i1}] \left[\phi_{j1}\right]}{d} \int\limits_0^l k_c(\hat{h}, \hat{c}) dx + \frac{[\phi_{i1}] \left[\phi_{j1}\right]}{d \int\limits_0^d \frac{dx}{k^\gamma(\hat{h}, \hat{c})}} \int\limits_0^d \frac{k_c^\gamma(\hat{h}, \hat{c})}{k^\gamma(\hat{h}, \hat{c})} dx,$$

$$f_i^{(11)} = \int\limits_0^l k(\hat{h}, \hat{c}) \frac{d\phi_{i1}(x)}{dx} dx + \frac{d\left[\phi_{i1}\right]}{\int\limits_0^d \frac{dx}{k^\gamma(\hat{h}, \hat{c})}},$$

$$m_{ij}^{(22)} = \int\limits_0^l \theta(\hat{h}) \phi_{i2} \phi_{j2} dx, \tilde{m}_{ij}^{(2)} = \int\limits_0^l \phi_{i2} \phi_{j2} dx, \tilde{f}_i^{(2)} = \int\limits_0^l c_0 \phi_{i2} dx, f_i^{(22)} = 0,$$

$$l_{ij}^{(22)} = \int\limits_0^l \theta(h) D(\hat{h}, \hat{c}) \frac{d\phi_{j2}}{dx} \frac{d\phi_{i2}}{dx} dx + \int\limits_0^l u \frac{d\phi_{j2}}{dx} \phi_{i2} dx +$$

$$+ (1 - \omega(\theta^-, c^-)) \frac{[\phi_{i2}] \left[\phi_{j2}\right]}{\int\limits_0^d \frac{dx}{\theta(h) D^\gamma(\hat{h}, \hat{c})}}.$$

4. Some practical aspects of the finite-element solving of the problem (1)–(10)

In practice, approximate finding of $h(x,t)$ and $c(x,t)$ utilizes the same net of finite elements. Then $\phi_{i1}(x)$, $\phi_{i2}(x)$, therefore to avoid double indexation, we denote these basis functions $\phi_i(x)$, $i = \overline{1, N}$. Similar to [25, 26], we cover $[0; \xi] \cup [\xi; l]$ with a finite-element grid. There are two finite elements in this case $[x_{m-1}; x_m] \in [0; \xi]$ and $[x_{m+1}; x_{m+2}] \in [\xi; l]$ such that $x_m = x_{m+1} = \xi$ and $x_m \in [0; \xi]$, $x_{m+1} \in [\xi; l]$. Basis functions $\phi_m(x)$ and $\phi_{m+1}(x)$ are discontinuous at $x = \xi$, i.e.

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

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

To simplify, time discretization is performed on a uniform grid with step τ. The number of steps in time is set as M. To find out $\mathbf{B}^{(p+1)}$, we perform

discretization of the system of non-linear differential equations (18) over time using a completely implicit linearized difference scheme [16]

$$\mathbf{M}_{22}(\mathbf{A}^{(p)}, \mathbf{B}^{(p)}) \cdot \frac{\mathbf{B}^{(p+1)} - \mathbf{B}^{(p)}}{\tau} + \mathbf{L}_{22}(\mathbf{A}^{(p)}, \mathbf{B}^{(p)}) \cdot \mathbf{B}^{(p+1)}$$

$$= \mathbf{F}_{22}(\mathbf{A}^{(p)}, \mathbf{B}^{(p)}), \ p = 1, 2, ...$$

where $\mathbf{A}^{(p)} = \mathbf{A}(t_p)$, $\mathbf{B}^{(p)} = \mathbf{B}(t_p)$, $t_p = p\tau$. After the formation of the linear system

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

where

$$\mathbf{G} = \frac{1}{\tau}\mathbf{M}_{11}(\mathbf{A}^{(p)}, \mathbf{B}^{(p)}) + \mathbf{L}_{11}(\mathbf{A}^{(p)}, \mathbf{B}^{(p)}),$$

$$\mathbf{F} = \frac{1}{\tau}\mathbf{M}_{11}(\mathbf{A}^{(p)}, \mathbf{B}^{(p)}) \cdot \mathbf{A}^{(p)} + \mathbf{F}_{11}(\mathbf{A}^{(p)}, \mathbf{B}^{(p)}),$$

we must take into account the principal boundary condition – the boundary condition of the first kind (2). This is accomplished by the following two steps: 1) all elements of the first equation of the linear system, including the free member, are nullified; 2) the first element of the first equation is set equal to 1, and the free member is set equal to $c(t_{p+1})$. The integrals in the formation of $\mathbf{G}$ and $\mathbf{F}$ are found by numerical integration. Similarly, $\mathbf{A}^{(p+1)}$ is found from (16) using obtained values $\mathbf{B}^{(p+1)}$.

5. Results of numerical experiments

Soil parameters for the numerical experiments are taken from the Hydrus-1D program [8]. As the main soil, loam with $k_0 = 0.028m/day$, $\theta_{\min} = 0.1$, $\theta_{\max} = 0.38$, $n = 1.23$, $\alpha = 2.7 \ day^{-1}$ were considered. As a soil of thin inclusion, clay with the following parameters was used: $k_0^\gamma = 0.0048 \ m/day$, $\theta_{\min} = 0.07$, $\theta_{\max} = 0.36$, $n = 1.09$, $\alpha = 0.5 \ day^{-1}$. The values of $R = 8.31446261815 \ J/mol \cdot K$, $T = 293.15K(20^0C)$, $M = 74.5513 \cdot 10$–$3kg/mol$, $\gamma = 104N/m^3$ were used. It was assumed that the main soil does not have osmotic properties, and that its ideality coefficient equals zero.

For the model problem, the layer of soil of $l = 3m$ thickness was considered. The depth of the inclusion was $\xi = 1.5m$, and its thickness $d = 0.2m$. The step of variable x was $0.005m$, the time step $\tau = 1day$. The starting distribution of heads was $h_0(x) = $ –$20m$. The original concentration of KCl in the chemical solution was $c_0(x) = 8mM$. The functions in the boundary conditions of the

first kind at the surface of the soil were $\overline{h}_0(t) = 0m$, $\overline{c}_0(t) = 400mM$. The results of the numerical experiments are presented in Tables 3-5.

Time moment	h^-	h^+	$[h]$	c^-	c^+	$[c]$
$t = 180 days$	0.3685	0.3319	-0.0366	41.82	47.92	-0.9
$t = 360 days$	0.3757	0.3556	-0.0201	94.80	65.91	-28.89
$t = 720 days$	0.3780	0.3674	-0.0106	198.80	151.12	-47.68
$t = 1080 days$	0.3800	0.3800	0	220.94	175.13	-45.81

Table 3. No semi-permeable properties of the clay inclusion ($\omega^\gamma = 0$)

Time moment	h^-	h^+	$[h]$	c^-	c^+	$[c]$
$t = 180 days$	0.3753	0.2651	-0.1102	38.78	20.65	-18.13
$t = 360 days$	0.3800	0.2668	-0.1132	69.92	17.73	-52.19
$t = 720 days$	0.3800	0.2591	-0.1209	116.21	23.24	-92.97
$t = 1080 days$	0.3800	0.3800	0	147.04	29.18	-117.86

Table 4. Consideration of osmosis and the ideality degree dependent on the KCl concentration

Time moment	h^-	h^+	$[h]$	c^-	c^+	$[c]$
$t = 180 days$	0.3731	0.2896	-0.0835	38.84	20.83	-18.01
$t = 360 days$	0.3761	0.3532	-0.0229	99.45	21.22	-78.23
$t = 720 days$	0.3777	0.3653	-0.0124	219.74	37.38	-182.36
$t = 1080 days$	0.3800	0.3800	0	271.07	48.18	-222.89

Table 5. Consideration only of the KCl concentration-dependent ideality degree and neglecting osmosis

The salt diffusion coefficient in the main soil was taken as [1]

$$D_1 |u| + \theta D_2 \tau_2$$

where D_1 is the hydrodynamic dispersion coefficient; D_2 is the molecular diffusion coefficient. According to [8, 18]

$$\tau_2 = \frac{\theta^{\frac{7}{3}}}{\theta^2_{\max}}.$$

For numerical experiments, aqueous KCl solution was considered as a chemical substance, with $D_2 = 1.721952 \cdot 10^{-5} \ m^2/day$ [21]. The hydrodynamic dispersion coefficient in this model problem was equal to the molecular diffusion coefficient. The KCl diffusion coefficient in a thin inclusion depended on the salt concentration according to the data of Table 1.

The results presented in Tables 3-5 show that both the semi-permeability and the inclusion of osmotic phenomena are essential in the predictive calculations. For instance, in the absence of the ideality of the geobarrier, the pollution level beyond the geobarrier after three years is already $175mM$ and differs from the level before the geobarrier only by $45mM$. When disregarding osmosis (Table 5), the pollution level beyond the geobarrier is $48mM$ which is much less than the results of the experiment according to Table 3. However, this is almost twice as high as for the case of the simultaneous consideration of the ideality degree and chemical osmosis (Table 4). Given that the process is long-term, the projected amount of contaminants transferred beyond the boundaries of the waste storage into ground water can vary considerably depending on the conditions for solving the problem. Therefore, it is important to take into full account the data of field observations and experiments in the model.

6. Conclusions

Thus, in this paper the mathematical model of the propagation of chemical substances in the soil that contains a thin clay geobarrier was investigated. The developed mathematical model takes into account: 1) the ideality properties of the barrier material; 2) the phenomenon of chemical osmosis; 3) the conjugation conditions account for the dependence of the filtration coefficient, the degree of ideality, the diffusion coefficient on the concentration of the chemi-cals. The numerical solution of the corresponding non-linear boundary value problem was found by the finite element method. The results of numerical experiments show that both the semi-permeability and the inclusion of osmotic phenomena are essential in the predictive calculations. For instance, in the absence of the ideality of the geobarrier, the pollution level beyond the geobarrier after three years differs from the level before the geobarrier only by 26%. When disregarding osmosis, the pollution level beyond the geobarrier differs from the level before the geobarrier by 463%. For the case of the simultaneous consideration of the ideality degree and chemical osmosis, the difference is about 400%. The numerical experments show the significance of considering chemical osmosis in the prediction calculations of the spread of harmful chemicals through geobarriers.

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