Methods of mathematical modeling and computer simulation were used to investigate the influence of interrelated processes of transfer of saline solutions in the unsaturated soil layer. To this end, a mathematical model has been built for modeling the corresponding processes of the moisture-, heat-, and mass transfer of saline solutions in an unsaturated soil layer. An effective computational algorithm was developed to solve the corresponding nonlinear boundary problem numerically by the method of finite differences; it was implemented in the Asp.net programming environment in the C++ language. Based on the numerical experiments carried out, the distribution of moisture, concentration, and temperature fields in the aeration zone (incomplete saturation) was obtained. To study the influence of mass transfer of salts on moisture transfer, a numerical solution was found to the problem of moisture transfer, the problem of moisture transfer taking into consideration mass transfer and moisture transfer, taking into consideration mass transfer in the presence of osmosis. Analysis of the results showed that the distribution of the concentration of saline solutions over time is slower and more predictable. It was established that the distribution of moisture heads increases with depth and time when saline solutions fall on the surface of the soil massif. With the influence of salt concentration, the distribution of moisture increases with depth and time throughout the entire area of moisture transfer by 1-3 %. The distribution of moisture heads taking into consideration the concentration of salts and osmosis is reduced by 3-5% compared to the results of the problem without taking into consideration the phenomenon of osmosis. The distribution of the concentration of saline solutions during moisture transfer and osmosis acquires higher values compared to the results without taking osmosis into consideration. The established features can be successfully applied to clean the fertile soil layer and resume agricultural activities

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Keywords: moisture-, heat-, and mass transfer, aeration zone (incomplete saturation), method of finite differences

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CONSTRUCTION OF A MATHEMATICAL MODEL AND NUMERICAL STUDY OF INTERACTION BETWEEN MOISTURE-, HEAT-, AND MASS TRANSFER PROCESSES OF SALT SOLUTIONS IN AN UNSATURATED SOIL LAYER

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1. Introduction

As a result of the negative influence of man-made factors, the biosphere is polluted, in particular fertile lands, with various kinds of salts and, specifically, radioactive substances. Accordingly, the urgent task today is to prevent contamination of groundwater and surface water, agricultural land; regulation of groundwater levels to avoid flooding of territories when hydrogeological conditions change and under the action of man-made factors. The process of filtration of saline solutions in soils is different from the filtration of pure water since the filtration of saline solutions in the soil is the movement of a weak electrolyte [1]. On the basis of experimental studies, patterns have been established that made it possible to update the known laws of Darcy, Darcy-Gersevanov, and Fick for the case of the movement of saline solutions in soils under non-isothermal conditions [2]. These studies were based on determining the dependences of the filtration characteristics of soils during the progress of moisture transfer, filtration, heat- and mass transfer in them. Based on the above, new mathematical models of salt solution filtration processes in catalytic and dispersed media of particles of microporous structure have been and built, and existing ones were updated, which more adequately describe the specified processes. That has made it possible to more accurately take into consideration the influence of various natural and manmade factors on the state of agricultural land. In the design and operation of hydro melioration systems in irrigated (drained) areas, the issues of studying the water-salt regime of soils and groundwater are of great importance. The main purpose of such research is to obtain better yields in agriculture and improve the resources of the soils themselves. Relevant studies are carried out with compatible processes in soils: filtration of saline solutions in a saturated area and moisture transfer in the area of incomplete saturation. For the same purpose, both ground and underground irrigation are used in land reclamation areas to stabilize irrigation moisture and fertilize the root layer of the soil, as well as and reduce their removal to groundwater.

Based on the foregoing and taking into consideration the importance, under modern conditions, of providing the population with environmentally friendly agricultural products, the task of studying the mutual influence of interrelated processes, such as moisture transfer, heat- and mass transfer in the aeration zone is relevant.

2. Literature review and problem statement

When modeling the process of moisture-, heat-, and mass transfer in porous media during groundwater filtration, the parameters of filtration and mass transfer (filtration coefficient, coefficient of convective diffusion, porosity) are considered constant in most cases. In this regard, the mass transfer of substances dissolved in water was mainly studied against the background of the filtration flow of groundwater, and instead of filtering the solution, pure water filtration was considered. However, a number of practical tasks (distribution of contaminants in soil arrays, filtration of saline solutions, etc.) revealed the inadequacy of existing mathematical models of the relevant processes. A large body of research into the issue of heat and mass transfer was reported in [3]; there, the classical development of heat transfer problems was exhaustively presented with a proper emphasis on understanding the physics of problems. However, the influence of heat exchange processes on others (moisture and mass transfer) was not taken into consideration. In [4], a three-phase model was built, capable of predicting heat transfer and moisture migration for the soil freezing process and heat and mass transfer mechanisms in unsaturated soil layers; the model developed in [4] was tested in [5]. Experimental research results were used for verification. The work also focuses on solving stationary and non-stationary two-dimensional thermal conductivity problems. For a more detailed research, refutation or confirmation of the hypothesis, more detailed studies of interrelated processes of heat-moisture and mass exchange processes are required. In [6], an improved thermohydraulic model for unsaturated freezing soils in cold regions was proposed; corresponding software based on the finite-difference method was developed. This model takes into consideration some physical processes, such as the curve of soil freezing characteristics and the depression of the freezing point. In addition, the rules for changing the content of non-frozen water and the total water content during the freezing process were analyzed. However, the focus was on exclusively low temperatures while in fact, it is necessary to consider the temperature regime in a wider range. The question of mathematical modeling and computer simulation of moisture-mass transfer in a one-dimensional case under non-isothermal conditions was partially addressed in [7, 8] but the interactions of the corresponding processes were not investigated. In [9], the problem of mathematical modeling of vertical migration of radionuclides in a catalytic porous medium under non-isothermal conditions was considered but the influence of moisture transfer on the corresponding process was not investigated. Some issues were tackled in [10] – the process of salt transport by filtration of saline solution and moisture transfer under the action of horizontal systematic drainage under the humidification mode, and in [11] - modeling the effect of infiltration on mass exchange processes in layered soils under heat transfer conditions. They considered somewhat specific issues relating to the processes of moisture-, heat-, and mass transfer, namely the migration of radionuclides and the transfer of salts; however, the attention was mainly focused on one of the processes (moisture-, heat-, and mass transfer). However, those processes are interrelated and can significantly affect one another. Therefore, it is worth considering those processes in complex interaction.

A fundamental and practical introduction to the use of computational methods, in particular methods of finite differences, in modeling fluid flows in porous media is set forth in [12]. This is the first book to cover a wide range of streams, including single-phase, two-phase, fuel oil, volatile, constituent, non-isothermal, and chemical constituent flows in both conventional porous and cracked porous media. In addition, a number of computational methods are used. In addition, providing a theoretical basis to engineers and scientists involved in modeling transfer processes in porous environments was the purpose of [13].

Consequently, the construction of new mathematical models and studying mutual influences of interrelated processes of moisture-, heat-, and mass transfer of saline solutions in the unsaturated soil layer deserves great attention.

3. The aim and objectives of the study

The aim of this study is to quantify the mutual influence of the processes of moisture-, heat-, and mass transfer of saline solutions in the unsaturated soil layer. This will make it possible to draw conclusions about the time of soil restoration providing for the possibility of further agricultural activities.

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

 to build a mathematical model of the processes of moisture-, heat-, and mass transfer of saline solutions in the unsaturated soil layer;

 to derive numerical finite-difference solutions to the corresponding nonlinear boundary problem for a system of differential equations;

- to conduct a series of numerical experiments and analyze them.

4. The study materials and methods

The study object of this work is the processes of moisture-, heat-, and mass transfer of salts of saline solutions in the unsaturated soil layer. There are a number of fundamental physical laws that describe the processes of mass transfer during the filtration of saline solutions in porous media. In particular, the generalized Darcy-Gersevanov law for the case of the movement of saline solutions in the presence of a temperature gradient takes the following form

 $\upsilon - e\mathbf{v} = -\mathbf{K}(c,T)\mathbf{C}h + \mathbf{v_c}\mathbf{C}c + \mathbf{v_T}\mathbf{C},$

where *e* is the coefficient of soil porosity; \mathbf{K} – coefficient (tensor) of filtration; *h* – head, \mathbf{v}_c , \mathbf{v}_T – coefficients (tensors) of chemical and thermal osmosis, respectively.

In this paper, it is assumed that the speed of movement of solid particles of the soil is zero.

Since under non-isothermal conditions there is a phenomenon of thermal diffusion and the specific flow of dissolved salts is defined as $q_c = \upsilon c - D(c,T)\nabla c - D_T \nabla T$, the equation for the transfer of salts in a porous medium takes the form (Fick's law)

$$\nabla \cdot \left(\mathbf{D} \nabla c \right) + \nabla \cdot \left(\mathbf{D}_{\mathbf{T}} \nabla T \right) - \left(\upsilon, \nabla c \right) = n_p \frac{\partial c}{\partial t},$$

where **D** is the coefficient (tensor) of convective diffusion; $\mathbf{D}_{\mathbf{T}}$ – coefficient (tensor) of thermal diffusion; v – filtration rate, which is determined according to the generalized Darcy-Gersevanov law; n_p – volume of pore solution per unit volume of soil; t – time.

Since the specific heat flux in the soil is defined as $q_{T} = \rho c_{\rho} \upsilon T - \lambda_{T} CT$, the heat transfer equation in a porous medium is as follows (Fourier's law)

$$\nabla \cdot (\lambda_T \nabla T) - \rho c_{\rho} (\upsilon, \nabla T) = c_T \frac{\partial T}{\partial t},$$

where λ_T is the coefficient (tensor) of the effective thermal conductivity of moist soil; ρ – density of saline solution; c_{ρ} – specific heat capacity of saline solution; c_T – volumetric heat capacity of the soil at a constant volume.

To find an approximate solution to the corresponding nonlinear boundary problems, numerical methods were used, namely a finite-difference method (FDM). As a result, we obtain the Cauchy problem for a system of nonlinear

first-order differential equations with respect to unknown functions that depend only on time. To find its (Cauchy's problem) solution, sampling schemes in time are used. In numerical experiments, piecewise-quadratic functions were used as basic functions of FDM, and a completely implicit linearized difference scheme was used as a sampling scheme in time.

5. Results of investigating the problem of mutual influence of the processes of moisture-, heat-, and mass transfer of saline solutions in the unsaturated soil layer

5. 1. Construction of a mathematical model of the processes of moisture-, heat-, and mass transfer of saline solutions in an unsaturated soil layer

Assume we have an extended soil massif, on the surface of which precipitation or irrigation falls with intensity e (Fig. 1). Over time, a groundwater level (GWL) is established at depth l, which is considered stationary, and a saline layer of soil is formed in a state of incomplete saturation (aeration zone). The distributions of moisture heads H_0 and concentra-

tion C_0 at the initial time t=0, their values on the soil surface H_1, \tilde{C}_1 , and GWL H_0, \tilde{C}_2 are known. The temperature regime of the soil massif changes over time. Temperatures $\tilde{T}_0(t)$, $\tilde{T}_1(t), \tilde{T}_2(t)$ are set in the soil layer, on its surface, and GWL, respectively. Under the influence of moisture transfer, the presence of gradients of salt concentration and temperature in the aeration zone, interrelated processes of transfer of moisture, salts, and heat occur.

Under the influence of moisture transfer, the presence of gradients of salt concentration and heat in the aeration zone, interrelated processes of transfer of moisture, salts, and heat occur. It is required to investigate the interrelated influence of the processes of heat and mass transfer of salts on moisture transfer, and vice versa, in the soil layer of great length. Namely: calculate the field of moisture heads in the aeration zone (incomplete saturation) and the field of concentrations and temperature in this zone over time. This will make it possible to make a forecast regarding the degree of soil purification and their further use.



Fig. 1. Moisture-, heat-, and mass transfer in an unsaturated layer of soil

The corresponding process will be considered under non-isothermal conditions under the influence (in the process) of vertical moisture transfer and concentration and temperature gradients in an unsaturated soil environment (aeration zone). As a result of the formalization of the above statement of the problem, the mathematical model of the interrelated processes of salt and heat transfer for a one-dimensional case, based on [9, 11], was written in the form of the following boundary problem:

$$\frac{\partial}{\partial x} \left(D(c,\Theta,T) \frac{\partial c}{\partial x} \right) - v(c,\Theta,T) \frac{\partial c}{\partial x} - -\gamma(c-C^*) + \frac{\partial}{\partial x} \left(D_T \frac{\partial T}{\partial x} \right) = \sigma \frac{\partial(\Theta c)}{\partial t},$$

$$x \in (0;l), \ t > 0, \tag{1}$$

$$\frac{\partial}{\partial x} \left(K(c,h,T) \frac{\partial h}{\partial x} \right) - - \frac{\partial}{\partial x} \left(v^T \frac{\partial T}{\partial x} \right) + f = \mu(h) \frac{\partial h}{\partial t},$$

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$$x \in (0; l), \quad t > 0, \tag{2}$$

$$\frac{\partial}{\partial x} \left(\lambda_T (c, \Theta, T) \frac{\partial T}{\partial x} \right) - \rho C_{\rho} \upsilon \frac{\partial T}{\partial x} = C_T \frac{\partial T}{\partial t},$$

$$x \in (0;l), t > 0, \tag{3}$$

$$v = -k(c,h,T)\frac{\partial h}{\partial x} + v\frac{\partial c}{\partial x} + v^{T}\frac{\partial T}{\partial x}, \quad x \in (0;l), \quad t > 0,$$
(4)

$$c(x,0) = \tilde{C}_{0}(x), \quad l_{1}c(0,t) = \tilde{C}_{1}(t),$$

$$l_{2}c(l,t) = \tilde{C}_{2}(t), \quad x \in (0;l), \quad t > 0,$$

$$h(x,0) = H_{0}(x), \quad h(0,t) = H_{1}(t),$$
(5)

$$h(l,t) = H_2(t), x \in (0;l), t > 0,$$
 (6)

$$T(x,0) = T_0(x), \quad T(0,t) = T_1(t),$$

$$T(l,t) = T_2(t), \quad x \in (0;l), \quad t > 0,$$
(7)

where $x \in [0; l] \ 0 < t < t_1, \ l_i = \overline{1,6}$ – differential operators that set boundary conditions at x=0 and x=l, respectively. The following designations are introduced here: c(x, t) – concentration of pore saline solution, D(c) – coefficient of convective diffusion, K(c) – coefficient of thermal diffusion,

$$\mu(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial x} (k(c,h,T)) - v \frac{\partial c}{xt}$$

- mass transfer coefficient, C^* - concentration of maximum saturation of saline solution, ρ , C_{ρ} - density and specific heat capacity of pore saline solution, k(c,h,T) - moisture transfer coefficient, h=P-x - moisture head, $P = \frac{p}{\rho g}$ - pressure height, v - moisture transfer rate, $\mu(h) = \frac{\partial \omega}{\partial h}$ - coefficient of soil moisture capacity at incomplete saturation, v, v^T - coefficients of osmosis and thermal osmosis, C_T - specific heat

capacity of the soil. Differential equations (1) to (3) and law (4) describe the following interrelated processes in an unsaturated soil layer (aeration zone):

(1) – convective diffusion (mass transfer) of saline solutions in the aeration zone (incomplete (P<0) saturation) under the influence of moisture transfer and thermal diffusion;

(2) – the process of moisture transfer under the influence of gradients of moisture pressure, salt concentration, and temperature (and $\mu(h)\neq 0$);

(3) – convective heat transfer under the influence of temperature and moisture gradients;

(4) – a generalized Darcy-Kluthe law for the case of moisture transfer under the influence of gradients of moisture head, salt solution concentration, and temperature. Boundary conditions (5) to (7) set the initial and boundary conditions, respectively, for concentration, pore moisture head, and soil temperature.

The boundary problem (1) to (7) is a system of three nonlinear one-dimensional parabolic equations with some initially unknown coefficients, which are derived later in the process of solving the boundary problem. 5. 2. Numerical solution to the problem of mutual influence of interrelated processes of moisture-, heat-, and mass transfer of saline solutions

To find the numerical solution to the boundary problem (1) to (7), a finite-difference method was used.

Entering a difference grid $W_{h_1h_2}$ with steps $h_1\tau$ along the Ox and Ot axes for variables x, t:

$$W_{h_{\mathrm{l}}\tau} = \left\{ \left(x_{i}, t_{k} \right) \middle| x_{i} = ih_{\mathrm{l}}, t_{k} = k\tau, i = \overline{1, n_{\mathrm{l}}}, k = \overline{1, n_{\mathrm{l}}} \right\},$$

where n_1 , n_2 is the number of steps for the spatial variable and time, respectively.

The difference scheme of the problem (1) to (7) is constructed as follows: for problem (2), (7), a purely implicit difference scheme is constructed [9], and for (1), (4), (5), and (3), (4), (7) – an improved monotonous finite-difference scheme [11].

In particular, the implicit difference scheme (1), (4), (5) takes the following form:

$$\mu_{i}^{k} \frac{H_{i}^{k+1} - H_{i}^{k}}{\tau} = \frac{1}{h_{1}} \left[a_{i+1}^{k} \frac{H_{i+1}^{k+1} - H_{i}^{k+1}}{h_{1}} - a_{i}^{k} \frac{H_{i}^{k+1} - H_{i-1}^{k+1}}{h_{1}} \right] - \nu \frac{C_{i+1}^{k+1} - 2C_{i}^{k+1} + C_{i-1}^{k+1}}{h_{1}^{2}} - \nu^{T} \frac{T_{i+1}^{k+1} - 2T_{i}^{k+1} + T_{i-1}^{k+1}}{h_{1}^{2}} + f, \qquad (8)$$

$$H_0^{k+1} = \phi_1^1 H_1^{k+1} + \mu_1^1, \quad H_n^{k+1} = \phi_2^1 H_{n-1}^{k+1} + \mu_2^1, \tag{9}$$

where

$$\begin{split} a_{i}^{k} &= 0.5 \Big(K \Big(H_{i}^{k}, C_{i}^{k} \Big) + K \Big(H_{i-1}^{k}, C_{i-1}^{k} \Big) \Big), \\ a_{i+1}^{k} &= 0.5 \Big(K \Big(H_{i+1}^{k}, C_{i+1}^{k} \Big) + K \Big(H_{i}^{k}, C_{i}^{k} \Big) \Big), \\ \mu_{i}^{k} &= a \rho g \Bigg(1 - \frac{2h_{1}}{H_{i+1}^{k} - H_{i-1}^{k}} \Bigg), \quad i = \overline{1, n_{1} - 1}, \quad k = \overline{0, n_{2} - 1}, \\ \chi_{1}^{1} &= \begin{cases} 0, h(0, t) = H_{1}(t), \\ 1, \frac{\partial h(0, t)}{\partial x} = 0, \\ 1, \frac{\partial h(0, t)}{\partial x} = 0, \end{cases} \chi_{2}^{1} &= \begin{cases} 0, h(l, t) = H_{2}(t), \\ 1, \frac{\partial h(l, t)}{\partial x} = 0, \\ 1, \frac{\partial h(l, t)}{\partial x} = 0, \end{cases} \chi_{2}^{1} &= \begin{cases} 0, h(l, t) = H_{2}(t), \\ 1, \frac{\partial h(l, t)}{\partial x} = 0, \\ 0, \frac{\partial h(0, t)}{\partial x} = 0, \end{cases} \chi_{2}^{1} &= \begin{cases} \tilde{H}_{2}^{k+1}, h(l, t) = H_{2}(t), \\ 0, \frac{\partial h(l, t)}{\partial x} = 0, \\ 0, \frac{\partial h(l, t)}{\partial x} = 0, \end{cases} \end{split}$$

The difference scheme (8), (9) was presented in the form:

$$a_{1}H_{i-1}^{k+1} - c_{1}H_{i}^{k+1} + b_{1}H_{i+1}^{k+1} = -f_{1},$$
(10)

$$H_0^{k+1} = \chi_1^1 H_1^{k+1} + \mu_1^1, H_n^{k+1} = \chi_2^1 H_{n-1}^{k+1} + \mu_2^1,$$
(11)

where

$$a_{1} = \frac{a_{i}^{k}}{h_{1}^{2}}, \quad b_{1} = \frac{a_{i+1}^{k}}{h_{1}^{2}}, \quad c_{1} = \frac{a_{i+1}^{k} + a_{i}^{k}}{h_{1}^{2}} + \frac{\mu_{i}^{k}}{\tau},$$
$$f_{1} = \frac{\mu_{i}^{k}}{\tau}H_{i}^{k} - \nu \frac{C_{i+1}^{k} - 2C_{i}^{k} + C_{i-1}^{k}}{h_{1}^{2}} - \nu \frac{T_{i+1}^{k} - 2T_{i}^{k} + T_{i-1}^{k}}{h_{1}^{2}},$$

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$$i = \overline{1, n_1 - 1}, \quad k = \overline{0, n_2 - 1}.$$

Numerical solution to (10), (11) was found by a double-sweep method [9]

$$H_i^{k+1} = \alpha_{i+1}^1 H_{i+1}^{k+1} + \beta_i^1, \tag{12}$$

where

$$\alpha_{i+1}^{1} = \frac{b_{1}}{c_{1} - \alpha_{i}a_{1}}, \quad \beta_{i+1}^{1} = \frac{a_{1}\beta_{i} + f_{1}}{c_{1} - \alpha_{i}a_{1}},$$
$$\alpha_{1}^{1} = 0, \quad \beta_{1}^{1} = \tilde{H}_{1}^{k+1}, \quad i = \overline{1, n_{1} - 1}, \quad k = \overline{0, n_{2} - 1}.$$

To solve the problem of mass transfer of salts (1), (4), (5), an improved (compared to [9]) monotonous difference scheme was applied [10].

The difference scheme of the set problem takes the following form [11]

$$\frac{1}{h_2} \left(\mu_{i2} d_{i+1}^k \frac{C_{i+1}^{k+1} - C_i^{k+1}}{h_1} - \mu_{i1} d_i^k \frac{C_i^{k+1} - C_{i-1}^{k+1}}{h_1} \right) + r_{i+}^k \frac{C_{i+1}^{k+1} - C_i^{k+1}}{h_1} + r_{i-}^k \frac{C_i^{k+1} - C_{i-1}^{k+1}}{h_1} + f^k = \Theta \frac{C_i^{k+1} - C_i^k}{\tau}, \quad (13)$$

$$C_i^0 = C_0(ih_1), \quad C_0^{k+1} = \chi_1^2 \tilde{C}_1^{k+1} + \mu_1^2, \quad C_n^{k+1} = \chi_2^2 \tilde{C}_{n-1}^{k+1} + \mu_2^2, \quad (14)$$

where

$$\begin{split} &d_{i}^{k} = \frac{D_{i}^{k} + D_{i-1}^{k}}{2}, \quad d_{i+1}^{k} = \frac{D_{i+1}^{k} + D_{i}^{k}}{2}, \\ &r_{i+}^{k} = 0.5 \Big(V_{i}^{k} + \left| V_{i}^{k} \right| \Big) \ge 0, \quad r_{i-}^{k} = 0.5 \Big(V_{i}^{k} - \left| V_{i}^{k} \right| \Big) \le 0, \\ &V_{i}^{k} = r_{i+}^{k} + r_{i-}^{k}, \quad \overline{f}_{2}^{k} = -\gamma \Big(C_{i}^{k} - C_{*} \Big) + D_{T} \frac{T_{i+1}^{k} - 2T_{i}^{k} + T_{i-1}^{k}}{h_{1}^{2}}, \\ &\mu_{i1}^{k} = \frac{1}{1 + \frac{0.5h_{1} \left| r_{i}^{k} \right|}{d_{i}^{k}}, \\ &\mu_{i2}^{k} = \frac{1}{1 + \frac{0.5h_{1} \left| r_{i}^{k} \right|}{d_{i}^{k}}, \quad i = \overline{1, n_{1} - 1}, \quad k = \overline{0, n_{2} - 1}; \\ &\chi_{1}^{2} = \begin{cases} 0, c(0, t) = C_{1}(t), \\ 1, \frac{\partial C(0, t)}{\partial x} = 0, \end{cases}, \quad \chi_{2}^{2} = \begin{cases} 0, c(l, t) = C_{2}(t), \\ 1, \frac{\partial C(l, t)}{\partial x} = 0, \end{cases} \\ &\mu_{1}^{2} = \begin{cases} \tilde{C}_{1}^{k+1}, c(0, t) = C_{1}(t), \\ 0, \frac{\partial C(0, t)}{\partial x} = 0, \end{cases} \\ &\mu_{2}^{2} = \begin{cases} \tilde{C}_{2}^{k+1}, c(l, t) = C_{2}(t), \\ 0, \frac{\partial C(l, t)}{\partial x} = 0, \end{cases} \end{split}$$

Erecting such members in (13), we received:

$$\begin{split} &\left(\frac{1}{h_2^2} \Big(d_i^k \mu_{i1}^k + d_{i+1}^k \mu_{i2}^k\Big) + \frac{\left|r_i^k\right|}{h_2} + \frac{\sigma}{\tau}\right) C_i^{k+1} = \frac{1}{h_2} \left(\frac{d_i^k \mu_{i1}^k}{h_2} - r_{i-}^k\right) \times \\ &\times C_{i-1}^{k+1} + \frac{1}{h_2} \left(\frac{d_{i+1}^k \mu_{i2}^k}{h_2} + r_{i+}^k\right) C_{i+1}^{k+1} + \frac{\sigma}{\tau} C_i^k + f_i^k. \end{split}$$

The difference scheme (13), (14) was represented as:

$$a_{2}C_{i-1}^{k+1} - c_{2}C_{i}^{k+1} + b_{2}C_{i+1}^{k+1} = -f_{2}^{k},$$

$$C_{i}^{k+1} - \alpha^{2}\tilde{C}_{i}^{k+1} + u^{2} - C_{i}^{k+1} - \alpha^{2}\tilde{C}_{i}^{k+1} + u^{2}$$
(15)

$$C_{0} = \chi_{1}C_{1} + \mu_{1}, C_{n} = \chi_{2}C_{n-1} + \mu_{2},$$

$$i = \overline{1, n_{1} - 1}, k = \overline{0, n_{2} - 1}.$$
 (16)

where

$$\begin{aligned} a_2 &= \frac{\mu_{i1}d_i^k}{h_1} - \frac{r_i^k}{h_1} \quad b_2 = \frac{\mu_{i2}d_{i+1}^k}{h_1^2} + \frac{r_{i+1}^k}{h_1}, \\ c_2 &= \frac{\mu_{i1}d_i^k}{h_1} + \frac{\mu_{i2}d_{i+1}^k}{h_1^2} + \frac{r_{i+1}^k}{h_1} - \frac{r_i^k}{h_1} + \frac{\Theta}{\tau}, \\ f_2^k &= \frac{\Theta}{\tau}C_i^k + \overline{f}_2^k, \quad i = \overline{1, n-1}, \quad k = \overline{0, K-1}. \end{aligned}$$

It can be shown that the conditions for the double-sweep stability $|\overline{c}_i^1| > |a_i^1| + |b_i^1|$ are met. As a result of solving the problem (15), (16) numerically, the concentration $c_1(x, t)$ on the time layer (*k*+1) was found by a double-sweep method [11], using the ratio

$$C_i^{k+1} = \alpha_{i+1}^2 C_{i+1}^{k+1} + \beta_{i+1}^2, \tag{17}$$

where

$$\alpha_{i+1}^2 = \frac{b_2}{c_2 - \alpha_i^2 a_2}, \quad \beta_{i+1}^2 = \frac{a_2 \beta_1^2 + f_2^k}{c_2 - \alpha_i^2 a_2},$$
$$\alpha_1^2 = 0, \quad \beta_1^2 = C_1^{k+1}, \quad i = \overline{1, n_1 - 1}, \quad k = \overline{0, n_2 - 1}$$

The improved monotonous difference scheme for (3), (4), (6) takes the following form

$$\frac{1}{h_{1}} \left(\overline{\mu}_{i2} \overline{d}_{i+1}^{k} \frac{T_{i+1}^{k+1} - T_{i}^{k+1}}{h_{1}} - \overline{\mu}_{i1} \overline{d}_{i}^{k} \frac{T_{i}^{k+1} - T_{i-1}^{k+1}}{h_{1}} \right) + \\
+ \overline{r}_{i+}^{k} \frac{T_{i+1}^{k+1} - T_{i}^{k+1}}{h_{1}} + \overline{r}_{i-}^{k} \frac{T_{i}^{k+1} - T_{i-1}^{k+1}}{h_{1}} = C_{T} \frac{T_{i}^{k+1} - T_{i}^{k}}{\tau},$$
(18)

$$T_{i}^{0} = T_{0}(ih_{1},0), T_{0}^{k+1} = \chi_{1}^{3}T_{1}^{k+1} + \mu_{1}^{3}, T_{n}^{k+1} = \chi_{2}^{3}T_{n-1}^{k+1} + \mu_{2}^{3},$$
(19)

where $\overline{d}_i^k = 0.5 \left(\lambda_{T,i}^k + \lambda_{T,i-1}^k \right)$,

$$\begin{split} \overline{d}_{i+1}^{k} &= 0.5 \left(\lambda_{T,i+1}^{k} + \lambda_{T,i}^{k} \right), \quad \overline{r}_{i+}^{k} &= 0.5 \rho C_{\rho} \left(\upsilon_{i}^{k} + \left| \upsilon_{i}^{k} \right| \right) \geq 0, \\ \overline{r}_{i-}^{k} &= 0.5 \rho C_{\rho} \left(\upsilon_{i}^{k} - \left| \upsilon_{i}^{k} \right| \right) \leq 0, \\ \overline{\mu}_{i1} &= \frac{1}{1 + \frac{0.5 h_{i} \left| \overline{r}_{i}^{k} \right|}, \quad \overline{\mu}_{i1} = \frac{1}{1 + \frac{0.5 h_{i} \left| \overline{r}_{i}^{k} \right|}, \\ 1 + \frac{0.5 h_{i} \left| \overline{r}_{i}^{k} \right|}{\overline{d}_{i+1}^{k}}, \quad \overline{d}_{i+1}^{k} = \frac{1}{1 + \frac{0.5 h_{i} \left| \overline{r}_{i}^{k} \right|}, \\ \chi_{1}^{3} &= \begin{cases} 0, T \left(0, t \right) = T_{1}(t), \\ 1, \frac{\partial T \left(0, t \right)}{\partial x} = 0, \end{cases} \quad \chi_{2}^{3} = \begin{cases} 0, T \left(l, t \right) = T_{2}(t), \\ 1, \frac{\partial T \left(l, t \right)}{\partial x} = 0, \end{cases} \\ \mu_{1}^{3} &= \begin{cases} T_{1}(t), T \left(0, t \right) = T_{1}(t), \\ 0, \frac{\partial T \left(0, t \right)}{\partial x} = 0, \end{cases} \end{split}$$

$$\mu_{2}^{3} = \begin{cases} T_{2}(t), T(l,t) = T_{2}(t), \\ 0, \frac{\partial T(l,t)}{\partial x} = 0, \end{cases}$$

The difference scheme (18), (19) is represented in the form:

$$a_{3}T_{i-1}^{k+1} - c_{3}T_{i}^{k+1} + b_{3}T_{i+1}^{k+1} = -f_{3}^{k},$$

$$T_{i}^{k+1} = \gamma^{3}T_{i}^{k+1} + \mu_{3}^{3}, \quad T_{i}^{k+1} = \gamma^{3}T_{i}^{k+1} + \mu_{3}^{3}.$$
(20)

$$i = \overline{1, n_1 - 1}, \quad k = \overline{0, n_2 - 1},$$
 (21)

where

$$a_{3} = \frac{\overline{\mu_{i1}}\overline{d_{i}^{k}}}{h_{1}^{2}} - \frac{\overline{r_{i}^{k}}}{h_{1}}, \quad b_{3} = \frac{\overline{\mu_{i2}}\overline{d_{i+1}^{k}}}{h_{1}^{2}} + \frac{\overline{r_{i+1}^{k}}}{h_{1}},$$

$$c_{3} = \frac{\overline{\mu_{i1}}\overline{d_{i}^{k}}}{h_{1}^{2}} + \frac{\overline{\mu_{i2}}\overline{d_{i+1}^{k}}}{h_{1}^{2}} + \frac{\overline{r_{i+1}^{k}}}{h_{1}} - \frac{\overline{r_{i}^{k}}}{h_{1}} + \frac{C_{T}}{\tau}, \quad f_{3}^{k} = \frac{C_{T}}{\tau}T_{i}^{k}.$$

It can be shown that the conditions for the stability of double sweep $|\overline{c}_i^4| > |a_i^4| + |b_i^4|$ are met. Numerical solution to (20), (21) was found by a double-sweep method

$$T_i^{k+1} = \alpha_{i+1}^3 T_{i+1}^{k+1} + \beta_{i+1}^3, \tag{22}$$

where

$$\alpha_{i+1}^{3} = \frac{b_{3}}{c_{3} - \alpha_{i}^{3} a_{3}}, \quad \beta_{i+1}^{3} = \frac{\alpha_{3} \beta_{1}^{3} + f_{3}^{k}}{c_{3} - \alpha_{i}^{3} a_{3}},$$

$$\alpha_{1}^{3} = 0, \beta_{1}^{3} = T_{1}^{k+1}, \quad i = \overline{1, n_{1} - 1}, \quad k = \overline{0, n_{2} - 1}.$$

The moisture transfer rate was found using the following difference ratio on the basis of (4):

$$V_{i}^{k} = -K_{i}^{k} \frac{H_{i+1}^{k} - H_{i-1}^{k}}{2h_{1}} + v \frac{c_{i+1}^{k} - c_{i-1}^{k}}{2h_{1}} + v_{T} \frac{T_{i+1}^{k} - T_{i-1}^{k}}{2h_{1}},$$

$$i = \overline{1, n_{1} - 1}, \quad k = \overline{0, n_{2} - 1},$$
(23)

Thus, the numerical solution to the boundary problem (1) to (7) has been algorithmically constructed in full.

5. 3. Results of numerical experiments and the analysis of the mutual influence of the processes of moisture-, heat-, and mass transfer of saline solutions

The software for the developed numerical method and the corresponding computational algorithms were implemented in the C++ programming language. As a result of software implementation, numerical solutions to individual problems that are included in the boundary problem (1) to (7) were obtained. The first is the problem of moisture transfer taking into consideration heat and mass transfer. The second is osmotic and thermal osmotic phenomena, convective diffusion taking into consideration moisture transfer and heat transfer, convective heat transfer taking into consideration moisture transfer.

Numerical experiments were carried out with the following initial data:

$$\begin{split} & T=360 \text{ days}, \tau=30 \text{ days}, l=15 \text{ m}, \sigma=0, \\ & \sigma_1=0.25, \gamma=0.0065 \text{ day}^{-1}, \\ & D_m=1\cdot10^{-6} \frac{\text{m}^2}{\text{day}}, \lambda=0.1 \text{ m}, \\ & \rho=1000 \text{ kg/m}^3, C_*=350 \text{ g/l}, \\ & \tilde{C}_0=10 \text{ g/l}, \quad \tilde{C}_1=0 \text{ g/l}, \quad \tilde{C}_2=0 \text{ g/l}, \\ & H_1=7 \text{ m}, H_2=20 \text{ m}, \\ & v=2.8\cdot10^{-5} \text{ m}^5/\text{kg}\cdot\text{day}, \\ & k_2(h_2)=\frac{a_1}{b_1+\rho^\alpha}=\frac{a_1}{b_1+\left[\rho g(h-x)\right]^2}, a_1=1, \\ & b_1=1, a_1=1, g=9.8 \text{ m/s}^2, \\ & D(c)=D_m+\lambda |V(x,c)|, \quad D_m=10^{-6} \text{ m}^2/\text{day}, \\ & l=10 \text{ m}, \quad \tilde{H}_1=1 \text{ m}, \quad \tilde{H}_2=0.1 \text{ m}, \\ & \gamma_1=\gamma_2=0.00065, k_f=1, R=1\cdot10^{-8} \text{ m}, \\ & D_2=1\cdot10^{-5} \frac{\text{m}^2}{\text{day}}, \quad D_0=1\cdot10^{-18} \frac{\text{m}^2}{\text{day}}, \\ & \tilde{C}_1^1(t)=5 \frac{\text{kg}}{\text{m}^3}, \quad \tilde{C}_1^2(t)=0 \frac{\text{kg}}{\text{m}^3}, \\ & \tilde{C}_2^1(t)=5 \frac{\text{kg}}{\text{m}^3}, \quad \tilde{C}_2^2(t)=0 \frac{\text{kg}}{\text{m}^3}, \\ & \tilde{C}_1^0(t)=5 \frac{\text{kg}}{\text{m}^3}, \quad \tilde{C}_2^0(t)=5 \frac{\text{kg}}{\text{m}^3}, \quad \tilde{Q}^0(x,r)=0 \frac{\text{kg}}{\text{m}^3}, \\ & c_\rho=4,2\cdot10^3 \frac{\text{J}}{\text{kg}\cdot\text{deg}}, \\ & c_r=2,137\cdot10^6 \frac{\text{J}}{\text{kg}\cdot\text{deg}}, \\ & \lambda_T=108\cdot10^3 \frac{\text{J}}{\text{m}\cdot\text{deg}\cdot\text{day}}, \\ & \tilde{P}_2(t)=5 \text{ °C}, \quad \tilde{T}_0(x)=1 \text{ °C}, \quad D_{T_1}=1\cdot10^{-4} \frac{\text{m}^2}{\text{day}}. \end{split}$$

The coefficient of convective diffusion was set linearly dependent on the filtration rate $D_{1,i}^{(k)} = D_{\mu} + \lambda |v_i^{(k)}|$, $i = \overline{1, n_1 - 1}$, $k = \overline{1, n_3}$, where D_{μ} is the coefficient of molecular diffusion in a porous medium, λ – the parameter of dispersion.

To conduct numerical experiments, the following dependence of the filtration coefficient on the concentration of saline solution and temperature was taken [14]:

$$k(c, t) = a_0 + a_1c + a_2c^2 + (a_3 + a_4c + a_5c^2)T + (a_6 + a_7c + a_8c^2)T^2$$

where *c* is the value of the concentration of the filtering solution; T – temperature; a – coefficients of the approximating function, defined as:

$$a_0 = -0.028, a_1 = 6.37 \cdot 10^{-4}, a_2 = -6.329 \cdot 10^{-7},$$

 $a_3 = 2.42 \cdot 10^{-3}, a_4 = -4.241 \cdot 10^{-5},$
 $a_5 = 7.744 \cdot 10^{-8}, a_6 = -2.306 \cdot 10^{-5},$
 $a_7 = 1.005 \cdot 10^{-6}, a_8 = -4.307 \cdot 10^{-9}.$

As a result of computer simulation, having conducted a series of numerical experiments, we constructed plots of the distribution of moisture heads (Fig. 2) and the distribution of moisture heads taking into consideration the concentration of salts (Fig. 3).



The distribution of moisture heads was found taking into consideration the phenomenon of osmosis on different time layers. Comparative plots of the results obtained take the following form (Fig. 4, 5).

Having found a solution to the problem of moisture transfer, a solution to the problem of mass transfer during moisture transfer and taking into consideration osmosis on different time layers was derived (Fig. 6, 7).

Fig. 6, 7 show the distributions of salt concentration, taking into consideration the heads of moisture and osmosis for 30 and 360 days.



Fig. 4. Distribution plot of moisture heads at T=30 days



Fig. 6. Plot of salt concentration distribution taking into consideration moisture heads and osmosis at T=30 days





6. Discussion of results of investigating the mutual influence of the processes of moisture-, heat-, and mass transfer of saline solutions

One can see from Fig. 2 that the distribution of moisture heads increases with depth and time. This is confirmed by a well-known fact, which is covered in many works [8-11]. When saline solutions get on the surface of the soil massif (Fig. 3), the influence of salt concentration on moisture distribution is clearly visible, which increases with depth and time throughout the entire area of moisture transfer by 1-3 %. This shows the effect of saline solutions on the process of moisture transfer. Fig. 4, 5 show the distribution of moisture heads taking into consideration the concentration of salts and osmosis. As can be seen, the moisture head decreases by 3-5 % compared to the results of the problem without taking into consideration the phenomenon of osmosis (Fig. 5). The effect of osmosis on the process of moisture distribution is negligible. Distribution of the concentration of saline solutions during moisture transfer and osmosis acquires higher values compared to the results without taking into consideration osmosis (Fig. 6, 7). In this case, the distribution of salt concentration increases in proportion to the choice of the osmosis coefficient or osmotic function; over time, the distribution of salt concentration stabilizes and gradually decreases (Fig. 7). This suggests that the osmotic phenomena affect the distribution of salt concentration in proportion to the choice of the osmosis coefficient with an increase in this coefficient, the distribution of salt concentration increases. The obtained features can be successfully used to clean the fertile soil layer and resume agricultural activities. However, in order to be able to carry out such calculations for real conditions, the hydrological characteristics of the soils must be known. This study will be advanced by increasing the dimensionality of the problem, improving models of moisture, heat and mass transfer of saline solutions in an unsaturated soil layer, and by proposing specific engineering solutions to change the osmotic effect on soil fertility.

7. Conclusions

1. A mathematical model of the processes of moisture-, heat-, and mass transfer of saline solutions in an unsaturated soil layer was constructed, which made it possible to build an effective computational algorithm for the numerical solution to the corresponding nonlinear boundary problem by a finite-difference method and to perform software implementation in the Asp.net programming environment in the C++ language.

2. Numerical finite solutions to the corresponding nonlinear boundary problem have been derived. Computer simulations have shown the mutual influence of interrelated processes of moisture, heat, and mass transfer of saline solutions in an unsaturated soil layer, in particular, that the effect of osmosis on the process of moisture distribution is negligible. The distribution of the concentration of saline solutions during moisture transfer and osmosis acquires higher values compared to the results without taking osmosis into consideration. Such influences should be taken into consideration in the study of agricultural areas. Assessment of the degree of such influences is the essence of a separate research task in the mechanics of porous media.

3. A series of numerical experiments were conducted to study the influence of interrelated processes of moisture-, heat-, and mass transfer. An increase in the distribution of moisture heads was established taking into consideration the concentration of salts in comparison with the problem of net moisture transfer by 3 %. The distribution of moisture heads taking into consideration the concentration of salts and osmosis is reduced by 3-5 % while the distribution to the choice of the osmosis coefficient or osmotic function.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

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