
About some features of forecasting masstransport processes in saturated - unsaturated media.

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ABSTRACT

The general methodic of forecasting the flow and moisture-salt transfer processes in saturated-unsaturated media on the base of the methods of mathematic modeling for case of the arbitrary vertical domains is proposed. The practical example of the solution the migration problem of pollutions at filtration from the irrigated channel to reservoir is demonstrated.

1. Introduction.

Geofiltration substantiation of complex measures to protect groundwaters from pollution used for drinking and industrial water supply as well as solving practical problems related to dissolution of salts, washing of saline soils and desalination of mineralized water requires the studying the processes transport of the salts and other polluting components by filtration flows in the zones of full and incomplete saturation of porous medium. At the same time the given problems of forecasting of the processes of flow and masstransfer may be solved effectively by the methods of the numerical

modeling. In proposed work the generalized methodic of mathematical modeling of the above processes for the cases of arbitrary vertical areas of filtration and migration of pollutions and a practical recommendations of its using for solutions the complex problems of environmental protection are presented.

2. The main part.

The problems of pollutions transport in saturated-unsaturated media are devoted the many works of the different authors [1,5-8,12-14]. As a rule in these works predicting the processes of mass transfer are considered relatively to the main component of salt transport on the base of conducted field and laboratory experimental works and that allows to simplify the mathematic model and the solution of the problem to the one-dimensional realization since the influence of the other components in processes of the migration in many cases may not be taken into account [6,12].

As it is known the mass flow \vec{q} in the migration of salts (salt groups) or individual ions is proportional to the gradient ΔC of concentration and the product of the velocity \vec{V} of the flow of moisture on the concentration C [1,7,12]:

$$\vec{q} = C\vec{V} - D\Delta C \quad (1)$$

where D – coefficient of molecular diffusion, m^2 / day .

For the scheme of a two-dimensional vertical flow the following mass salinity conservation equation can be recorded without taking into account the mass transfer between the salts of the solution and the salts in the rock (in the solid phase):

$$\frac{\partial(Q_1 C)}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial z} \left(D \frac{\partial C}{\partial z} \right) - \frac{\partial}{\partial x} (C V_{x_s}) - \frac{\partial}{\partial z} (C V_{z_s}) \quad (2)$$

where Q_1 – volume of water per unit volume of soil; $D = D_M + \lambda |\vec{V}|$ – coefficient of convective diffusion; D_M – coefficient of molecular diffusion; λ – coefficient of dispersion; C – mass concentration of salts (ions) per unit volume of solution, g / l .

At this the waterbearing horizons are assumed to be homogeneous and isotropic, the fluid is not compressed and the fluid motion is two-dimensional in the plane xOz . The z -axis is facing up; $F_z(x)$ – surface of the earth; $F_u(x, z) = 0$ – the boundary of the unpermeable layer; w_1, w_2 – respectively

zones of full and incomplete saturation; $F_H(x, z)$ - separating of their free surface boundary; w_{01}, w_{02} - low-permeable layers whose properties allow them to be considered as the waterunpermeable layers; w^+ - an area that complements the investigated one to a rectangular(Fig.1).

In each of the allocated zones w_1 and w_2 the motion of water is described by the laws of preservation of the masses and Darcy-Klyuta [5,7,12]:

$$\frac{\partial Q_s}{\partial t} = -\left(\frac{\partial}{\partial x}(Vx_s)\right) + \left(\frac{\partial}{\partial z}(Vz_s)\right) + w(x, z, t, Q) \quad (3)$$

$$Vx_s = -K_s \frac{\partial}{\partial x}(\psi + z), \quad Vz_s = -K_z \frac{\partial}{\partial z}(\psi + z) \quad (4)$$

where $\psi = \rho / \delta g$, $\delta = const$ - liquid density; ρ - pressure; $w(x, z, t, Q)$ - a member that characterizes the uptake of moisture by the roots of plants and moisture condensation.

Functions $Q_s(\psi)$ and $K_s(Q)$ are given for $\psi < 0$ and $Q < Q_2 < Q_1$ and are continuous and such that $Q_1 = Q_2(0)$, $0 < K(Q_2) < K_1$, $K_1(Q_1) = K_1 = const$, $\psi < 0$ - in the zone incomplete saturation, $\psi > 0$ - in the zone of full saturation; on a free surface $F_H \quad \psi = 0$.

Study of moisture flows in an unsaturated media requires an additional experimental studies in relation $Q_2 = Q(\psi)$, $K_2 = K(Q_2)$. For different types of soils and ranges of changes ψ these dependencies are represented in the scientific literature by different dependencies for example [5,9,12]:

$$\overline{Q_2} = \frac{Q_2 - Q_0}{Q_n - Q_0} = e^{\delta\psi} \quad (5)$$

$$K(\overline{Q_2}) = K_1(\overline{Q_2})^n, \quad K_1 = const \quad (6)$$

where Q_n, Q_0, δ, n - parameters determined experimentally for a specific soil.

If we use the Hawyside function $\xi(\psi)$ and expressions $\partial Q_2 / \partial \psi = f_2$, $(\overline{Q_2})^n = f_1$ and taken above assumptions with respect to the parameters of the flow of moisture in the w area we can write the equation describing the couple movement of water in the saturated-unsaturated zone as :

$$\begin{aligned} \xi(-\varphi)f_1(\psi) \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial x} \left[K_1(\xi(\psi) + \xi(-\psi)f_2(\psi)) \frac{\partial \psi}{\partial x} \right] + \\ + \frac{\partial}{\partial z} \left[K_1 \left(\xi(\psi) + \xi(-\psi)f_2(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right) \right] + w(x, z, t, Q_2) \end{aligned} \quad (7)$$

For $f_2(\psi) = 0$ the equation (7) will have the following form:

$$\mu \delta(\psi) \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial x} \left[K_1 \xi(\psi) \frac{\partial \psi}{\partial x} \right] + \left[K_1 \xi(\psi) \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] + W \frac{\partial}{\partial z} (\xi(\psi)) \quad (8)$$

where μ - water deficiency or lack of saturation, $\delta(\psi)$ - Dirac's function.

Using of the more general expressions than (5) - (6) in relation to the functions Q and $K(Q)$ gives rise to a more reasonable transition from (7) to (8) and to consider equation (8) as a special case of equation (7) in the assumption that in the zone of incomplete saturation the absence of a flow is determined by zero parameters Q and $K(Q)$.

Equations (2), (7) and (8) allow us to consider unilateral processes of convective diffusion without taking into account the mixing of solutions, etc. The account of local moisture inputs to the surface F_z , the flow of moisture and salts during irrigation are taken into account in the boundary conditions or by the introduction of an additional members in equations (2), (7), (8). Failure to calculate the aeration zone (region w_2) in the equation (2) and the additional w^+ region is accomplished by setting the zero values of convective diffusion D , the velocities of the moisture transfer V_{x2} , V_{z2} and the initial zero values of ψ . On the boundaries of the filtration area w_1 the natural conditions of the first and second kind are given and on the boundaries of the additional domain w^+ the natural conditions of non-leakage (the second kind).

Since equation (8) refers to equations of a parabolic type then to its numerical implementation it is expedient to use purely implicit differences schemes [10].

The proposed method reduction of the flow of any configuration to a rectangular and the need to use a large number of input information assumes the use of the finite difference methods, implicit schemes and the uneven discretization of the filtration area [10]. At this the equation (7) is replaced by a system of nonlinear algebraic equations taking into account the different boundary conditions with using iterative methods for the solution of algebraic equations [6,7,12].

Taking into account the slow down nature of passing the processes of salt transport in time in comparison with the processes of moving the moisture in the soils for the discretization of the equation (2) on a rectangular grid a purely explicit schemes were used with the check of the stability conditions at each step in time τ_k . From here the equation (2) is replaced in the nodes of a non-uniform rectangular grid of the region $\{w_k\}$ by a differential-difference analogue of the following form:

$$\begin{aligned} & \frac{1}{2} S_z \left[\left(CVx_s - D \frac{\partial C}{\partial x} \right)_{i-Y_2,j} + \left(CVx_s + D \frac{\partial C}{\partial x} \right)_{i+Y_2,j} \right] + \\ & + \frac{1}{2} S_x \left[\left(CVz_s - D \frac{\partial C}{\partial z} \right)_{i,j-Y_2} + \left(-CVz_s + D \frac{\partial C}{\partial z} \right)_{i,j+Y_2} \right] + w_{ij} = \frac{\partial}{\partial t} (QC)_{ij} \frac{S_{ij}}{4} \end{aligned} \quad (9)$$

where h_{xi}, h_{zj} – grid steps; $S_{ij}=S_x \times S_z$ – the area of a separate block of a discrete area of filtration w ; $S_x=h_{xi}+h_{xi+1}$; $S_z=h_{zj}+h_{zj+1}$, $Y_2 = 1/2$.

The approximation of the boundary conditions of the second kind is performed analogously by introducing fictitious nodes of the grid and taking into account the differential operator of the equation (2). For example for the left boundary node $\left(\frac{\partial \psi}{\partial x} = 0 \right)$ we can write:

$$\begin{aligned} & \frac{1}{2} S_z \left[\left(-CVx_s + D \frac{\partial C}{\partial x} \right)_{i+Y_2,j} \right] + \frac{1}{2} S_x \left[\left(CVz_s - D \frac{\partial C}{\partial z} \right)_{i,j-Y_2} + \left(CVz_s + D \frac{\partial C}{\partial z} \right)_{i,j+Y_2} \right] = \\ & = \frac{\partial}{\partial t} (QC)_{ij} \frac{S_{ij}}{4} \end{aligned} \quad (10)$$

Derivatives in the expressions (9)-(10) are replaced by the finite differences through of the values of the function $C_{i,j\pm 1}, C_{i\pm 1,j}$ in the nodes of the grid taking into account the direction of the filtration flow that is the signs of velocities Vz_s, Vx_s in order to obtain a positive definite difference operator [4,5,10].

In accordance with the adopted discrete scheme of equation (2) the derivative of time $\frac{\partial}{\partial t}$ is replaced in (9)-(10) in accordance with the explicit scheme [10,12].

The solution of the difference problem at each time step is carried out in two stages :

In the first stage the difference equation of motion of moisture is solved under the implicit scheme at given τ_k which results in the calculation of the value of velocities $(Vx_s)_{ij}, (Vz_s)_{ij}$ in each node of the grid that are the output information for solving the difference equations of salt transfer.

In the second stage in accordance with the explicit difference equations (9)-(10) the values of the total concentration $C_{ij,ke}$ in the nodes of the grid are calculated with the simultaneous verification of the stability condition which consists of in choosing such a step in time τ_{KC} at which the difference operator of the equation (2) remain to be positively defined. In the opposite

case the step τ_{KC} is reduced by the number of integers $\frac{\tau_K}{\tau_{KC}} = m_\tau$ and the calculation of concentration $C_{ij,ke}$ occurs at each step $\tau_K m_\tau$ times. The choice m_τ is performed for each particular case and depends on the stability conditions of the difference problem for equation (2) and the choice of step τ_k for equation (7).

The proposed methodic was used for the solution of the practical problem of mass transfer for conditions characteristic to hydrogeological and land reclamation situation in the territory of the Kherson region [2,3,11]. The transient filtration in a three-layer aquifer with almost horizontal roof and a sole of separate layers is considered (Fig.1). The initial position of the free surface of the filtration stream corresponds to the level of groundwaters in the upper layer with parameters $K_1 = 15 \text{ m / day}$, $\mu = 0,18$. The coefficients of filtration and water yield of the lower and middle layers are respectively taken $K_3 = 6 \text{ m / day}$, $\mu_3 = 0,2$, $K_2 = 0.005$, $\mu_2 = 0.05$. The linear dimensions of the filtration area are shown in Fig.1. With increase in one of the distribution channels of the Irrigation System the water level the filtration flow was directed towards the reservoir with a lower level of water in it which in turn caused the migration of salts in this direction. In modeling the process of salt transport the following output parameters were set: the values of the diffusion coefficients respectively in the upper, middle and lower layers - 0,01, 0,001, 0,005 m^2 / day ; the value of the parameters of the moisture transfer $Q_n = 0,52$, $Q_0 = 0,2$, $n = 2$, $\delta = 1,2 (1 / \mu)$. The rate of moisture transfer (evaporation) on the surface of the earth was given constant and equal to 0.002 m / day . The initial values of mineralization in the studied filtration areas were set variable only in the horizontal direction (axis X) from 0.4 to 3.0 g / l and in the vertical direction (Z axis) were set constant. Solution of the problem consist in the determination of the time of stabilization of convective transfer of salts in the aquifer after rise in the water level in the left channel of 0.1 m and at displacement of the boundaries of saline waters with mineralization from 1.0 to 2.0 g / l . In Fig.1 the solid lines show the initial isolines of equal concentrations before increases the water level in channel and the dotted isolines show isolines of concentration after the stabilization of the convective transfer ($t = 4.5$ years). The results of the calculations showed that the maximum displacement of the isoline of equal concentration $C = 1 \text{ g / l}$ is 100 m and $C = 2 \text{ g / l}$ - 200 m. From behind the lower filtration properties of the impermeable layer the impact of the lower aquifer on the process of the salt transfer in upper layer is absent practically and for the design calculations it is possible not to use it.

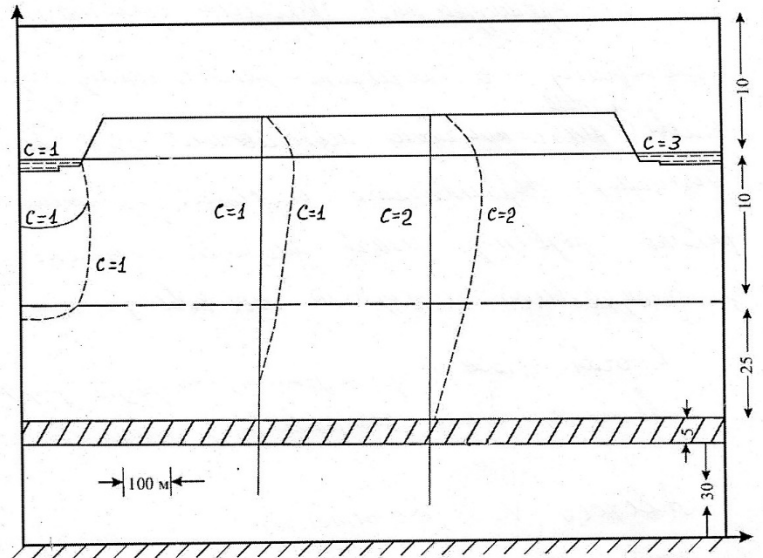


Fig.1. Results of solution the problem of salt transport between irrigated channel and reservoir for the case of the water level changing in channel on 0.1m.

Obviously that at further rising of the water level in channel the front of displacement will be moved to the right border of flow domain until to reach a new stabilization position.

Conclusions

Developed methodic of solution two-dimensional mass transport problems in saturated-unsaturated media in the domains of arbitrary forms allows to work on the complex tasks of prediction the processes of pollutions migration on irrigated lands and build-up territories. In some cases solution of above problems by the numerical modeling is more trustworthy and substantiate in comparison with using of the one-dimensional analytic ones. Presented results of solution of the practical problem show on the wide possibilities of using the proposed methodic.

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