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THE METHODIC OF CALCULATIONS OF THE CONTAMINATION OF THE GROUND WATERS ON THE IRRIGATED LANDS AND THE AJOINED TERRITORIES

***Abstract.** The general methodic of calculations of the contamination spreading of the different origin in the ground waters on the irrigated lands and ajoined territories on the base of the modern mathematical models of the masstransfer is proposed. Some features of the calculation models and the criterias of its using are analysed. The methodic example of the analytic solution of the masstransfer problem for the case of the homogeneous watersaturated media is presented.*

***Key words:** contamination; masstransfer; filtration; sorbtion; diffusion; dispersion; irrigation; mathematic models; base calculative schemes*

Introduction

The substantial changing of the biosphere and its individual components caused by intensive technogeneous influence on the surrounding media in modern conditions presents a serious threat to environmental safety and requires the immediate adoption of the adequate measures. In particular many environmental experts notice a dangerous trends in development the environmental conditions in rural areas where the extensive approach to agriculture negatively affected on the land fund [2–4]. Soil depletion by reducing total reserves of nutrients and worsening of the its structural properties due to the gradual destruction of aggregates and the impoverish ment of the composition of the microflora are complicated by the processes of erosion, flooding and salinization that occurring almost everywhere and therefore the most reliable way of improving of the productivity and preserving of lands lies in the profound investigations of a soil regimes [2, 4].

Not long ago it has come to the common opinion that obtaining maximum yields should not be the determining purpose of agrarian policy [4]. Indeed, its achievement is usually associated with a high risk of the spreading of toxic compounds of nutrients (nitrites, nitrates) outside the regulated area (field) and their accumulation in plant production. Using of contaminated with such compounds production causes poisoning, metabolic disorders, chronic diseases and other even more serious health problems in the population [1, 4, 11]. To our mind the only reliable means to prevent migration and accumulation of biogenic toxins consist of in creation a modern methodological base with a broad involvement the data of the natural experiments with the following profounded analysis of its. This requires an in-depth study of the soil processes and the substantiation of the basic soil regimes, the construction of a generalized mathematical models and the development of the methods for calculating regime characteristics, constructive and technological parameters [13, 14].

The main features of proposed methodic

The key point in any theoretical analysis of the behavior of the ecosystems soil-plant is a complex model of nutritional regime which in each case has a complicated structure dictated by high requirements for the quality of scientific predictions and is due to the diversity of nutrients and regime-forming processes (transformational, exchange, transport) [4, 6, 7].

Thus the models of water regime should necessarily to reflect the features of the flow of groundwater with full and incomplete saturation as a single stream consisting of two zones with significantly different water-physical properties and include the main water-physical characteristics of moisture – the main hydrophysical characteristics and the coefficient moisture transfer which in full saturation is coefficient filtration [1, 6, 7].

In general the decisive role in the construction of calculative models of migration based on which the hydrogeochemical prediction, planning and interpretation of regime observations are carried out is played the migration schematization of the processes and conditions of mass transfer in aquifers [6, 9, 10]. In this case two stages can be distinguished: 1) filtration schematization of migration conditions; 2) schematization of the process of mass transfer (actually the migration schematization). It should be noted that the first stage in the general case is not equivalent to the geofiltration schematization carried out in relation to the substantiation of the models of the geofiltration process. In addition we note that a fairly clear separation of two stages of migration schematization is possible only under conditions where the filtration pattern does not depend on the transport of matter. The main aspects of migration schematisation are as follows:

- 1) schematization of the influence of processes of mass transfer on the calculation schemes of filtration;
- 2) schematization of physico-chemical interaction of groundwater with the main body of the soil as well as physical and chemical transformations occurring directly in the underground solutions;
- 3) revealing of the relative importance of the individual mechanisms of convective-dispersive transfer;
- 4) substantiation of the appropriate levels of the study of migration processes in heterogeneous aquifer systems with the analysis of the possibilities of the reduction of heterogeneous complexes to quasihomogeneous;
- 5) schematization of the structure of the migration flow;
- 6) schematization of the boundary conditions of migration;
- 7) schematization of the development of the migration process in time.

Schematization of the effect of mass transfer on the calculation scheme of filtration should proceed primarily to assess the possible impact of migrating components on the density and to a lesser extent the viscosity of groundwater. If the changes in these indicators are markedly small then as a rule the filtering part of the migration task can be considered independently of the mass transfer. It should be noted that the set of conditions in which it is possible to neglect changes in the density of groundwater depend heavily on a particular filtration picture first of all from the gradient of the stream J and its orientation as well as from the profile filtration anisotropy.

In schematization of physico-chemical processes the general assumptions are reduced to the following: 1) thermodynamic conditions are often considered constant regardless of the migration process; 2) the migration of each of the components is considered independently without taking into account their mutual influence (both in the solution and in the mineral phase); 3) although for the aquifers solutions the

variety of chemical states of elements contained in them is typical all estimates are made only for prevailing migration forms with known thermodynamic parameters.

Despite the fact that these assumptions in many cases are idealized they are still widely used in practice due to the weakness of other approaches and the difficulties of their implementation and the lack of their trustworthy input information.

The greatest interest from the positions of possible simplification of the calculation model is the estimation of the relative importance of the convective transfer on the one hand and the diffusion- dispersion on the other. To do this you can use the ratio of the size of the transition zone (due to hydrodispersion) and the characteristic length of the transfer as well as known estimates which are given in the different publications [1, 6–10].

Schemes that neglect the hydrodispersion (schemes of piston extrusion) provide a safety margin for estimating concentration values along filtration flow trajectories that coming from a source of pollution but at the same time lowering the time of the initial stage of pollution and the size of the area covered by pollution. Possibility of widespread use of the schemes of piston extrusion (only convective transfer) is not in doubt when assessing the ascending inflow of deep mineralized water to drainage: the effect of hydrodispersion here is noticeably smoothed by the simultaneous tightening of solutions to water intakes from various hydrochemical zones.

The primary aspect of the migration schematization of the flow structure is the construction of a real often three-dimensional process of transferring a neutral component to two-dimensional or one-dimensional models which is achieved by fragmentation of the process in space and time. In the analysis of such a possibility and ways of its realization it is necessary to consider together many factors among which the main ones are: 1) the degree of development of the transverse (plan and profile) dispersion; 2) heterogeneity of the medium; and 3) characteristic distances and transport time.

In the first (and partly in the third) of these factors it is necessary to allocate in first of all the migration flows with a noticeable and neglectably small development of the planned transverse dispersion; such differentiation is determined mainly by the filtration field near the source of pollution and the characteristic length of the transfer L as well as the intensity of the dispersion. In the case of not too large values of L and with a sufficiently high hydrodynamic activity of the source in comparison with the estimated flow of the natural filtration flow the first type of migration flows develop "areas of spreading" in which the transverse plan dispersion can be neglected. So for the axial line of the area this is assumed already when the next criterion is fulfilled: $Q_0 > (5...10)Q_e / \sqrt{L/\delta'}$, where δ' is the parameter of the transverse dispersion. On the contrary rather length migration flows from the sources with comparatively weak hydrodynamic activity are related to the second type "areas of scattering". Here the value of the transverse plan dispersion is usually large (at least for the times of order $t_0 = Ln/V_e$). By analogy it is possible to write the following necessary criterion for the area of scattering taking into account the transverse dispersion: $Q_0 < (1...2)Q_e / \sqrt{L/\delta'}$.

For flows of the first type the basic calculative estimates can be made along the fixed lines of flows in the plane without taking into account the interaction between them. In this case the profile two-dimensional or even one-dimensional calculation models of migration can be used.

For the flows of the second type due to the need to take into account the transversal plane dispersion the calculative migration model should be two-dimensional in the plane. Within the framework of this model the profile heterogeneity of aquifers can also be taken into account provided that the field of the filtration rates in the profile is one-dimensional within the selected elements of the layer. Otherwise it is necessary to appeal to three-dimensional migration models which at the modern conditions is not real.

Analyzing the formulation of the boundary conditions of migration it should be noted that for layers of small length when the main features of the migration process are quickly determined by the influence of the original boundary it is unacceptable to carry out the schematization based on field estimates for the calculative models of an unbounded layer. This circumstance has the fundamental importance to scattering areas. In this case the presence of a remote external boundary and the nature of the conditions on it can radically change the concentration field not only near the boundary but also at considerable distances from it. At intensive removal of matter from the boundaries (the first kind) a general tendency towards to decreasing in concentration appears and at the zero condition of the second kind there is a tendency of the opposite direction.

We especially note the need for direct account in the boundary conditions the migration parameters of the rocks and man-made formations with the special properties distinctive to the supply contours (for example the pools of industrial wastes).

When schematising the development of the migration process in time in the general case it is necessary to focus on the non-stationary statement of the problem of mass transfer. As exceptions there are the scattering areas that are formed in the intensive manifestation of the transverse dispersion. For such areas it is significant the formation of the stationary (quasi-stationary) migration fields near the entry boundaries that gradually increase in size over the time.

It should be noted that the principles of migration schematization differ substantially more higher complexity than the usual principles of geofiltration schematization and only in some cases can be reduced to the strict quantitative criteria. On the other hand in the study of the migration processes as a rule the shortage of necessary source information is much more affected and the main limiting factor is often the lack of substantiation of the filtration scheme.

Migration of fertilizers, pesticides and other pollutants in the irrigation areas under the conditions of interconnection of underground and surface water is formed under the influence of permanently operating sources of dissolved pollution (canals, rivers) as well as pollutants that coming from the zone of aeration during irrigation from the surface of the earth when fertilizers and pesticides are introduced and the peculiarities of this process are caused by various parameters relations.

An analysis of the conditions of the motion of various fertilizers, pesticides and other substances in groundwater on irrigated areas under the conditions of interconnection of underground and surface waters allows to distinguish several typical schemes that are most commonly encountered in migration studies [8, 9].

So in Fig. 1 the scheme of filtration and migration of contaminants from the canal and from the irrigated lands in the reservoir (river) is presented which is one of the most typical. In this case the waterdivide is not present and the migration of pollution occurs in one direction.

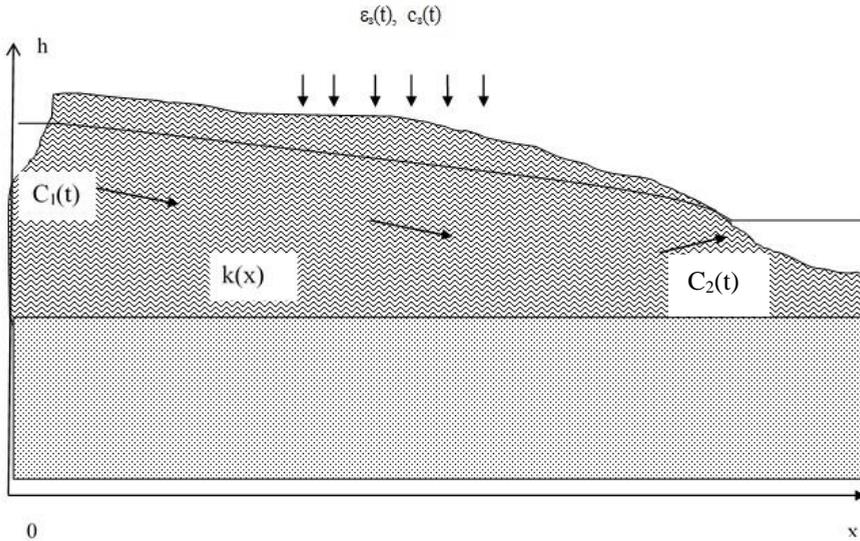


Fig. 1 – Scheme of filtration and spread of contamination from the canal and from irrigated land to the reservoir (pond)

$C_1(t)$, $C_2(t)$ – concentration of pollution in the channel and the reservoir (river),
 $C_p(t)$ – concentration of contaminants in irrigation water,
 $\varepsilon(t)$ – Infiltration power intensity,
 —→ – the direction of the spread of contamination

The equation of motion and the preservation of the mass of salts for the above scheme can be written as [1, 5, 8]:

$$-\frac{\partial q}{\partial x} + \varepsilon_1 C^* - \varepsilon_2 p C = \frac{\partial(nhC)}{\partial t} \quad (1)$$

$$q = \left(vC - D \frac{\partial C}{\partial x} \right) h, \quad D = D_m + \lambda |v| \quad (2)$$

where q – mass flow of salts in the ground water stream; D – coefficient of convective diffusion; C – concentration of salts in any section of the flow; C^* – concentration of salts that come with the infiltrated water; p – normalization factor; λ – dispersion parameter; D_m – coefficient of molecular diffusion; v – velocity of the filtration flow.

Coefficient $p = 1$ if the evaporating moisture from the groundwater surface contains volatile components of salts and $p = 0$ if not contains.

The equation (2) can be represented as follows:

$$\begin{aligned} \frac{\partial}{\partial x} \left(Dh \frac{\partial C}{\partial x} \right) + C \left(-\frac{\partial v h}{\partial x} + \varepsilon - m_0 \frac{\partial h}{\partial t} \right) - \\ - v h \frac{\partial C}{\partial x} + \varepsilon (C_p - C) = m_0 h \frac{\partial C}{\partial t} \quad (3) \\ \varepsilon = \varepsilon_2 p + \varepsilon_0; \quad c_p = \varepsilon_1 C^* / (\varepsilon_2 p + \varepsilon_0) \end{aligned}$$

If the evaporation from the groundwater surface is absent or not taken into account ($\varepsilon_2 = 0$) then $C_p = C^*$, $\varepsilon = \varepsilon_0 = \varepsilon_1$. If the ground waters are high and the evaporation has a place then at $p = 0$ will be $c_p = \varepsilon_1 C^* / \varepsilon_0$ and $\varepsilon = \varepsilon_0$ and if $p = 1$ respectively $C_p = C^*$ and $\varepsilon = \varepsilon_1$.

Based on the equation of continuity the second component in equation (3) is assumed to be 0.

Then taking into account the variable values of the filtration rate, the thickness of the flow and the mass transfer processes equation (3) can be written as:

$$\frac{\partial(nC)}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial C}{\partial x} \right) - V \frac{\partial C}{\partial x} + \frac{\varepsilon}{h} (C_p - C) - \frac{\partial \sigma}{\partial t} \quad (4)$$

where σ – mass concentration of the substance in the solid phase.

The above differential equations allow us to find the fields of the concentrations in groundwaters when we know the distribution of the concentrations at the initial moment of time (initial conditions), the geometric form of the considered filtration domain and the velocity field in it and also the conditions for salt exchange at the boundaries of this domain (boundary conditions) and experimental parameters of salt transfer (coefficients of the differential equations) which are using from the experimental research.

We can write these conditions for the systems of equations (1)–(3). Initial conditions are determined by the distribution of the contaminations concentrations in the soil at some point in time adopted at the beginning of the reference time of the process ($t = 0$). In the initial concentration state of the medium the entire previous history of the process is reflected and for the subsequent course of the changing in the salt process it does not matter at all how this conditions arose.

Mathematically the initial conditions can be expressed by the dependencies of the form:

$$C(x,0) = C^0(x) = f_1(x), \quad \sigma(x,0) = \sigma^0(x) = f_2(x) \quad (5)$$

Schematization is used to simplify the problem of solving when the uneven initial distribution of pollution is replaced by averaging.

It should be noted the peculiarity of the boundary value problems of salt transfer in soils: the longer the time passes from the initial moment the less initial conditions affect the concentration fields.

Boundary conditions (at $x = 0$) can be as follows:

1. On the boundaries of the domain may be given a condition of the first kind for example on the boundary of the waste waters reservoir in the inlet section ($x = 0$)

$$C(0,t) = C_s(t) \text{ or } C_s = \text{const} \quad (6)$$

where C_s – concentration of water in the storage, g/l.

2. More often the boundary condition of the third kind formulated for the first time by Dankworth is given at the entrance boundary ($x = 0$)

$$(C(0,t) - C_p)V = D \frac{\partial C(0,t)}{\partial x} \quad (7)$$

This condition expresses the balance of dissolved pollutions in the inlet section of the flow: the flow of pollutants entering to the soil due to filtration is equal to the pollution discharge at the lateral boundary layer ($x = 0$) which is formed as a result of diffusion and filtration. Using this condition gives a gradual change in concentration near the lateral boundary of the layer to the concentration C_p which is observed in the real conditions of migration of pollutions.

At the outer boundary of the layer at ($x = L$) the boundary condition of the second kind is most often set.

The following system of equations is used to simulate the migration of contaminations in the ground waters taking into account the lateral source of chemical elements (river, canal) and their arrival on a free surface from the surface of the earth (irrigated and rainy land).

At this assumed that the filtration flow in two-layer domain for example is nonstationary and the values of the filtration rates in each of the layers V_1, V_2 are obtained from solving of the problem of nonstationary filtration. Then we have the following system of the equation:

$$n_1 \frac{\partial C_1}{\partial t} = \frac{\partial}{\partial x} \left(D_1 \frac{\partial c_1}{\partial x} \right) - V_1 \frac{\partial C_1}{\partial x} - \lambda C_1 - \frac{\partial \sigma_1}{\partial t} - \frac{D_1}{m_s m_1} (C_1 - C_2) + \frac{\varepsilon}{m_1} (C_p - C_1) \quad (8)$$

$$\frac{\partial \sigma_1}{\partial t} = \alpha_1 C_1 - \beta_1 \sigma_1 \quad (9)$$

$$n_2 \frac{\partial C_2}{\partial t} = \frac{\partial}{\partial x} \left(D_2 \frac{\partial c_2}{\partial x} \right) - V_2 \frac{\partial C_2}{\partial x} - \lambda C_2 - \frac{\partial \sigma_2}{\partial t} + \frac{D_1}{m_s m_2} (C_1 - C_2) \quad (10)$$

$$\frac{\partial \sigma_2}{\partial t} = \alpha_2 C_2 - \beta_2 \sigma_2 \quad (11)$$

where x – horizontal coordinate; t – time; $C_1(x,t)$ – concentration of the pollutions in the pore solution in the upper layer; $C_2(x,t)$ – the concentration of the same contaminations in the pore solution in the lower layer; $\sigma_1(x,t)$ – concentration of solid phase contaminations in the upper layer; $\sigma_2(x,t)$ – concentration of contaminations in the solid phase in the lower layer; n_1, n_2 – active porosities of each layer; λ – the rate of destruction (decay) of a substance determined by the properties of pollution and therefore is the same for each of the layers; α_i ($i = 1,2$) – coefficients of adsorption rate of matter in each of the layers; β_i ($i = 1,2$) – coefficients of the rate of desorption of matter in each of the layers; D_1 – diffusion coefficient; m_1, m_2 – the thickness of the upper and lower layers; m_s – the thickness of the separator layer; ε – intensity of infiltration; C_p – concentration of contaminations in the infiltration water.

To solve the equations (8)–(11) the initial and boundary conditions are defined that correspond to the peculiarities of the simulated processes.

So if the flow of contaminations into the formation occurs on the left border at $x=0$ and the aquifer is drained on the right border at $x=L$ then the boundary conditions can be written as:

$$C_1(x,0) = C_1^0, \quad C_2(x,0) = C_2^0, \quad \sigma_1(x,0) = \sigma_1^0, \quad \sigma_2(x,0) = \sigma_2^0, \quad (12)$$

$$(C_2(0,t) - C_{2,p})V_2 = D_2 \frac{\partial C_2(0,t)}{\partial x} \quad (C_1(0,t) - C_{1,p})V_2 = D_1 \frac{\partial C_1(0,t)}{\partial x} \quad (13)$$

$$\frac{\partial C_2(L,t)}{\partial x} = \frac{\partial C_1(L,t)}{\partial x} = 0 \quad (14)$$

It should be noted that the above equations with the corresponding initial and boundary conditions can be solved by well known numerical methods and the methods of the finite differences are used most often [1, 5, 8, 11, 12]. However for the study and analysis of the above processes in many cases it is sufficient to consider simplified models that can be realized by the analytical methods.

As was already noted above it is too hard to obtain a solution of the equations of migration of pollutions even in the conditions of homogeneous soil if taking into account the changeability of the input coefficients and the arbitrary boundary conditions.

However with the large values of the Peckle parameter (at neglecting of the diffusion transport of the matter) the constant values of the coefficients of equations, the constant initial and boundary conditions the mathematical model of migration in a homogeneous soil (4)–(6) can be simplified and reduced to the consideration of the next system of equations:

$$n \frac{\partial C}{\partial t} = -V \frac{\partial C}{\partial x} - \lambda C - \frac{\partial \sigma}{\partial t} + \frac{\varepsilon}{m} (C_p - C), \quad (15)$$

$$\frac{\partial \sigma}{\partial t} = \alpha C. \quad (16)$$

with initial conditions

$$C(x,0) = C^0, \quad (17)$$

$$\sigma(x,0) = \sigma^0. \quad (18)$$

and a boundary conditions

$$C(0,t) = C_L. \quad (19)$$

For analytical solution of the given system the method of Laplace's integral transformations was used [1, 8].

After obvious transformations and direct using of Laplace's inverse transformation we obtain the next formula for determining the first of two unknown functions $C(x, t)$:

$$C(x, t) = \left[\left(C_L - C^0 \frac{k_2}{k_1} \right) e^{-\frac{n}{V} k_1 x} - C^0 \left(1 - \frac{k_2}{k_1} \right) e^{-k_1 t} \right] \eta \left(t - \frac{nx}{V} \right) + \frac{C^0 k_2}{k_1} + C^0 \left(1 - \frac{k_2}{k_1} \right) e^{-k_1 t}. \quad (20)$$

A solution for another unknown function $\sigma(x, t)$ is obtained from the second equation of the output system of equations by direct integration and in the result of the obvious transformations as:

at $t < \frac{nx}{V}$

$$\sigma(x, t) = \alpha \frac{C^0 k_2}{k_1} t + \frac{\alpha C^0}{k_1} \left(1 - \frac{k_2}{k_1} \right) (1 - e^{-k_1 t}), \quad (21)$$

at $t \geq \frac{nx}{V}$

$$\sigma(x, t) = \frac{\alpha C^0 k_2}{k_1} t + \frac{\alpha C^0}{k_1} \left(1 - \frac{k_2}{k_1} \right) \left(1 - e^{-k_1 \frac{nx}{V}} \right) + \alpha \left(C_L - C^0 \frac{k_2}{k_1} \right) e^{-\frac{n}{V} k_1 x} \left(t - \frac{nx}{V} \right). \quad (22)$$

It is easy to verify that the obtained solutions (20)–(22) satisfy the equations as well as the initial and boundary conditions.

The results of the analytical calculations of the methodic problem with using the equations (20)–(22) for the case of the lateral and infiltration contaminations of the ground water taking into account the sorption for the following input data: $\varepsilon = 0,003$ m/day; $m = 20$ m; $n = 0.3$; $\alpha = 0,0002$ 1/day; $\lambda = 0.001$ 1/day; $C^0 = 0,5$ mg/l; $C_L = 5$ mg/l; $C_P = 5$ mg/l; $S^0 = 2.5$ mg/dm³; $V = 0.1$ m/day are shown in Fig. 2.

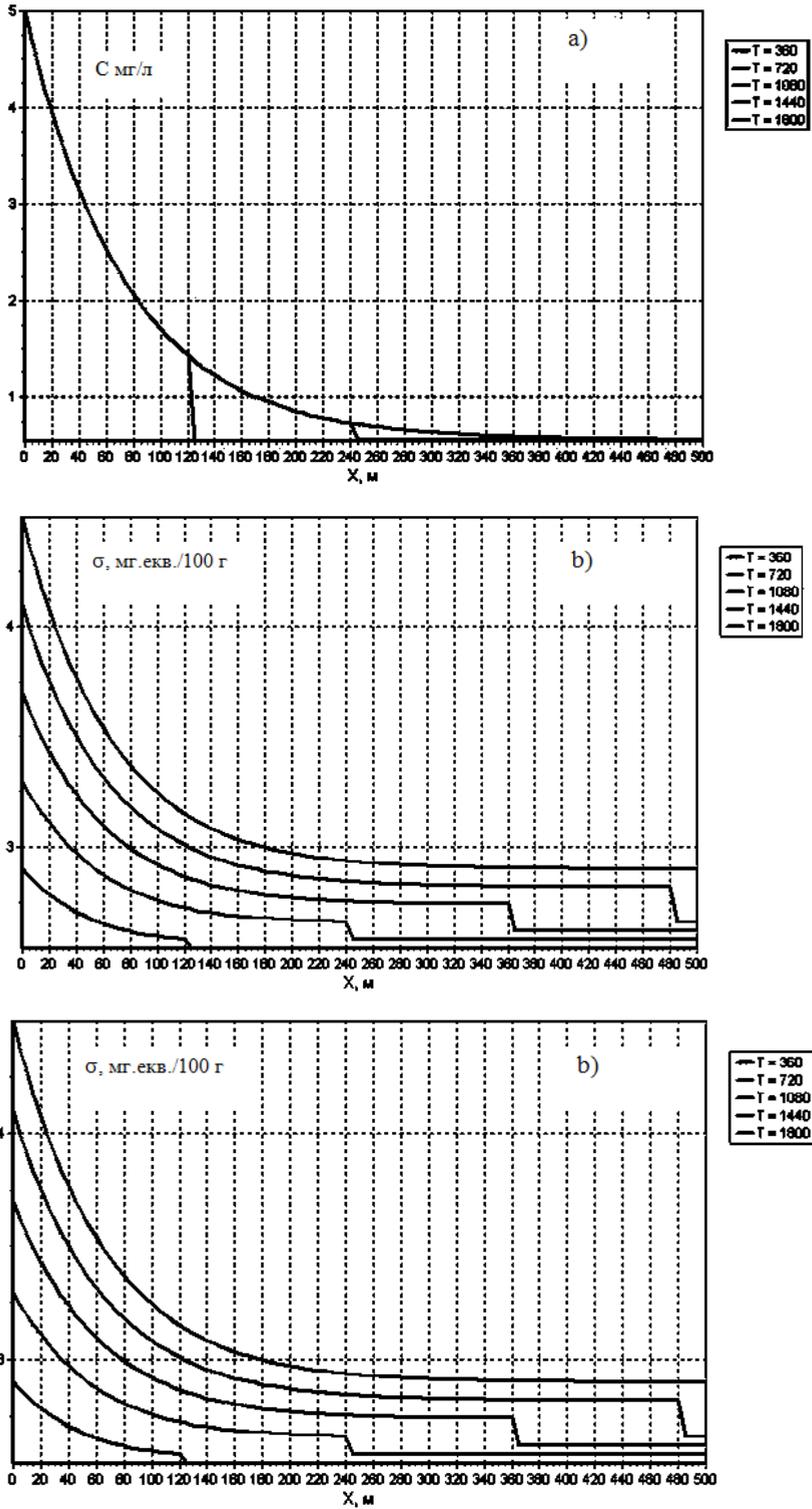


Fig. 2 – Graphs of the dependences of the concentrations of the contaminations in the solution (a) and adsorbed on the soil particles along the length of the filtration area (b) at different times

As can be seen under given conditions a case of the contaminations or desalinization close to the piston superseding scheme is realized but both to the boundary of the "piston" and after it the concentrations of the contaminations are monotonously changed which is associated with the manifestation of sorption and degradation mechanisms and the quantitative values of concentrations are determined with the interdependency of the values of the input parameters. As a result such solution has an approximate character and for it improving it is necessary to use the numerical methods of the calculation. The using of the numerical methods of the solutions for more complex problems of the contaminations of the water media on the base of the considered above mathematical models of the mass transfer is presented in some works [5, 8, 9].

Conclusions

Using of proposed methodic and models allows to consider the processes of contamination of ground water for many cases on the substantial scientific level and to realize of the solution of the wide spectrum practice problems for protection from pollution of the water media in different regions including the irrigated lands and adjoining territories.

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МЕТОДИКА РОЗРАХУНКІВ ЗАБРУДНЕННЯ ҐРУНТОВИХ ВОД НА ЗЕМЛЯХ ЗРОШЕННЯ ТА ПРИЛЕГЛИХ ТЕРИТОРІЯХ

Анотація. Запропонована узагальнена методика розрахунків розповсюдження забруднень різного походження в ґрунтових водах на землях зрошення та прилеглих територіях на основі сучасних математичних моделей масопереносу. Проаналізовано деякі особливості розрахункових моделей та критерії їх застосування. Наводиться методичний приклад аналітичного розв'язку задачі масопереносу для випадку однорідного водонасиченого середовища.

Ключові слова: забруднення; масоперенос; фільтрація; сорбція; дифузія; дисперсія; зрошення; математичні моделі; основні розрахункові схеми

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