NUMERICAL SIMULATION OF RAINWATER RUNOFF OVER CATCHMENT SURFACE AND MASS TRANSFER OF CONTAMINANT INCOMING TO WATER STREAM FROM SOIL

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ABSTRACT
The subject of an article is the mathematical and numerical modeling of the rainwater runoff along the surface catchment taking account the transport of pollution which permeates into the water flow from a porous media of soil at the some area of this surface. The developed mathematical model consists of two types of equations: the equations for calculating of the water layer thickness over the slope surface given the precipitation and evaporation, and equation of the mass transfer of impurity coming into the surface water during its filtration in zone of incomplete saturation of soil. The model also takes into account a reverse process – adsorption of impurity in soil with its low concentration or in the uncontaminated soil. Water content in the zone of incomplete saturation is determined within the approximate approach based on the model of capillary impregnation. The principal features of the problem solution are theoretically studied. In particular, it is shown that the equation for water content in this zone can become a differential equation with lagging argument. Computational schemes to solve the system of nonlinear differential equations are developed with the finite-difference methods using a priori information about the solution behavior. The numerical model is implemented in the software for computer simulation of the processes with simultaneous graphic visualization of the computing results. The numerical model is implemented in the computer software for simulation and simultaneous graphic visualization migration both the rain water and contaminant in the river basin.
Keywords: Numerical Simulation, Rainwater Runoff, Transfer of Contaminant, the Surface Catchment, Sorption, Desorption, Zone of Incomplete Saturation, Capillary Impregnation
1. INTRODUCTION

The investigation of the interrelated mass transfer in the rainwater runoff along the catchment surface and in the porous media of soil in the basin of rivers is of central interest for hydrology, hydrogeology, environmental geology and other allied sciences. Surface runoff has annual periodicity, however, its creation and behavior can significantly vary in depend on the intensity of precipitation, evaporation, absorption of water in the entire area of the catchment and many other factors (Anderton, 2002; Beven, 1984; Beven, 1979). These processes are further complicated by the presence of the contaminated areas with soil containing the various types of pollution which can permeate into runoff due to desorption of contaminant from the pores of soil into the water flow. There can arise also a reverse process - adsorption of impurity in soil with its low concentration or in the uncontaminated soil.

Runoff is associated with the following three types of flow: the surface flow (continuous or consisting of set of streamlets), a subsurface runoff and a groundwater runoff. Subsurface runoff has a relatively high speed in the inclined upper layers of soil, for example, at filtration of water and its motion through macro-pores and cracks. The rate of water movement along the slope beneath the catchment surface, on the one hand, is significantly less than on this surface. On the other hand, it is much more than the filtration velocity in the aquifers.

Groundwater runoff is the water flow along the saturated aquifers to the river network. This flow represents only a small part of the river hydrograph although some amount of water can come into the river channel immediately after rainfall. In various physical and geographical areas (Dunne, 1975; Eagleson, 1970; Hewlett, 1967) and even within watersheds of relatively small sizes, the runoff formation may be caused by a variety of factors. Often runoff transforms from one form to another and these changes depend on the surface relief, types of atmospheric fallout, their intensity and total amount (Jost et al, 2007; Luce et al, 1998; Pomeroy et al, 1998; Pomeroy, 1996, 1997, 1998; 1998, 2002; Talbot, 2004; Winkler et al, 2005).

The behavior of runoff and migration of contaminant along the catchment surface, the riverbed and its feeders can be investigate with mathematical modeling (Antontsev...
Computation of the interrelated processes during a motion of rainwater, groundwater and contaminant in the river basin is characterized also by a large amount of input data, including boundaries of watershed and areas of contamination, the topography the catchment surface given the depth of the river network, etc. Grid data may be prepared using any standard geoinformation systems and the number of the grid nodes usually amount to hundreds of thousands and tens of millions. In such situations the computational efficiency can be significantly improved with the special numerical schemes and modern methods of parallel computing on multiprocessor computers. So the objective of this work is extension of mathematical model and numerical methods (Konyukhov et al, 2013; Konyukhov et al, 2013) in case of the pollutant transport by the rainwater runoff.

2. MODEL OF THE RUNOFF AND MASS TRANSFER OF IMPURITY

Mathematical model of the rainwater runoff along the surface catchment was developed earlier in our previous papers (Konyukhov et al, 2013; Konyukhov et al, 2013) in framework of the concept of two-dimensional kinematic wave. To describe the mass transfer of contaminant incoming to the water stream from the porous media of soil, this model was modified and amplified with new equations. In result, new generalized system equations can be written as following:

$$\frac{\partial (U + \Theta)}{\partial t} + V_x + V_y = \varepsilon_1, \quad V_x = -U^{5/3}V_{1,x}, \quad V_y = -U^{5/3}V_{1,y},$$

(1)

$$\frac{\partial (CU)}{\partial t} + \frac{\partial (CV_x)}{\partial x} + \frac{\partial (CV_y)}{\partial y} = \beta - C \frac{\partial \Theta}{\partial t}, \quad h(1-m)\frac{\partial C}{\partial t} = h\beta ,$$

(2)
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\[
V_{i,x} = \frac{Z'_i}{n\sqrt{\nabla Z}}, \quad V_{i,y} = \frac{Z'_y}{n\sqrt{\nabla Z}}, \quad |\nabla Z| = \sqrt{Z'^2_x + Z'^2_y}, \quad Z = H + U,
\]

(3)

\[
\Theta = \sqrt{a^2 t^2 + bt + at}, \quad a = 0.25 mg pr^2 / \mu, \quad b = 0.5m^2 \sigma r \cos \alpha / \mu,
\]

(4)

\[
\beta = \begin{cases} 
0, & \text{if } u > 0, \\
\lambda (C_x - C), & \text{if } H(x, y) \leq u > 0,
\end{cases}
\]

\[
\beta_s = \begin{cases} 
0, & \text{if } \partial \Theta / \partial t = 0, \\
\gamma (C_x - C_y), & \text{if } \partial \Theta / \partial t > 0.
\end{cases}
\]

Here \( x \) and \( y \) are spatial coordinates; \( t \) is the time; \( U(x, y, t) \) is the thickness of the water layer at the catchment surface; \( \Theta(x, y, t) \) is water content in coil within zone of incomplete saturation («ZIS»); \( m \) is the porosity of this area; \( C(x, y, t) \) is the impurity concentration in water solution of the surface flow; \( C_s(x, y, t) \) is the similar characteristic of the water solution in the soil thin boundary layer, by which water enters the soil from earth surface; \( h \) is the thickness of boundary layer; \( V(x, y, t) \) is the velocity vector of the surface flow; \( H(x, y) \) is the ground elevation above sea level; \( n \) is the roughness coefficient of the catchment surface; \( \varepsilon_i(x, y, t) \) is the function that specifies amount of precipitation and evaporation; \( \rho \) is the water density; \( g \) is the gravity acceleration; \( r \) is the average radius of pores in zone of incomplete saturation; \( \sigma \) is the surface tension coefficient; \( \alpha \) is the wetting angle; \( \mu \) is the viscosity of water solution; \( \beta(x, y, t) \) is desorption of impurity from the surface of pores in soil by rainwater; \( \beta_s(x, y, t) \) is the amount of the desorbed impurity in water, moving in the porous medium, per unit volume of soil; \( \lambda \) and \( \gamma \) are coefficients of desorption; \( Z_s = \partial Z / \partial x; \ Z_y = \partial Z / \partial y \).

System of differential equations (1) – (4) governs the mass transfer in the catchment area \( D \) with boundary \( \Gamma = \Gamma_w + \Gamma_r \), where \( \Gamma_w \) is the watershed line; \( \Gamma_r \) is intersection of this line and the river surface at its lower course, see Fig. 1. Initial and boundary conditions are:
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\[ U(x, y, 0) = 0, \quad C(x, y, 0) = 0, \quad V_n|_{\Gamma_w} = 0, \quad C_s(x, y, 0) = \begin{cases} 0, & (x, y) \notin D_c, \\ C_s^0(x, y), & (x, y) \in D_c. \end{cases} \]

(5)

Here \( V_n|_{\Gamma_w} \) is the normal velocity at the boundary \( \Gamma_w; D_c \) is the area of contamination source with the initial concentration \( C_s^0(x, y) \).

**Note 1.** Parameter \( h \) in the second equation (2) can be used as a verification parameter of model. It can be defined by computations in the every concrete situation. In the simplest case we can put \( h = 1 \). Further, since absorption goes much faster than desorption so we can assume that the impurity concentration in the water solution at its moving along this thin layer is the same as in the water solution coming from the surface. In this case \( \beta_s = \beta_s(C, C) \), and the desorbed impurity is instantly transported by water flow throughout the length of ZIS.

Note 2. If surface-water flow brings the impurity to the area with its lower concentration or to the area free from contaminant then the reverse process (the sorption) takes place.

Fig. 1. Topographical relief of the river basin, the bed of the river with inflows and area \( D \) of the runoff formation in the presence of water pollution zone \( D_c \) in the soil

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in soil with coefficients $\lambda$ and $\gamma$, which values differ from values of $\bar{\lambda}$ and $\bar{\gamma}$, so that

$$
\begin{align*}
\lambda &= \begin{cases} 
\lambda, & C_s \geq C, \\
\bar{\lambda}, & C_s < C,
\end{cases} \\
\gamma &= \begin{cases} 
\gamma, & C_s \geq C, \\
\bar{\gamma}, & C_s < C.
\end{cases}
\end{align*}
$$

**Note 3.** In the model (1) – (4) the impurity concentration in ZIS is not computed, however at each point $(x, y) \in D_c$ the total amount $\delta q(x, y, t)$ of contaminant gone with the water stream in the time interval $[0, t]$ is defined as $\delta q = \int_0^t (\beta - C \partial \Theta / \partial t) dt$. It is obvious that the value $\delta Q = \int_{D_c} \delta q dxdy$ is equal to amount of impurity which gone away from the area $D_c$.

### 3. Principal Features of the Differential Equations Solution

Important features of the searched solution of equation (1) were studied in our work (18) in absence of impurity in the rainwater runoff. Now we generalize and reformulate obtained earlier results for the case of presence of contaminant in soil, ingress of impurity into water and its moving with the surface flow.

3.1. Since there is no inflow through the boundary $\Gamma_w$ of the watershed, so the thickness $U$ of the liquid layer in the area $D$ becomes greater than zero only due to the function $\varepsilon_1$, characterizing the intensity and the duration of rainfall. At the same time, water soaks into the soil in zone of incomplete saturation with the flow rate which is determined by the derivative $\partial \Theta / \partial t$. If precipitations have small intensity, then the pores of ZIS can completely absorb all rainwater. The absence of the surface runoff in the area $D$, i.e. equality to zero of the functions $U(x, y, t)$, reflects the inequality

$$
\varepsilon_1 \leq \frac{\partial \Theta}{\partial t} = \frac{a^2 t + b / 2}{\sqrt{a^2 t^2 + bt}} + a,
$$

which follows from equation (1) and relationship (4).
3.2. Let us consider the equation (1) at the initial time, i.e. for $t \to 0$. The surface runoff can only arise if it rains, so the limit $\varepsilon_i \big|_{t \to 0}$ tends to the defined finite value $\varepsilon_i^0$. On the other hand, $t = 0$ is the time appearance of an instant water source on the boundary of zone of incomplete saturation. The discharge flow of this source is determined by the value $\partial \Theta / \partial t \big|_{t \to 0}$. At $t \to 0$ one obtains $\partial \Theta / \partial t \big|_{t \to 0} \approx (2a + 0.5\sqrt{b/t}) \to \infty$.

(7)

Thus, in the initial time the condition (6) is fulfilled, and surface runoff is formed not at once but only after some time. In addition, as it follows from relation (7), the surface-water flow is missing at $\varepsilon_i \leq 2a$ regardless on duration of precipitation. Note, that from the physical standpoint the parameter $2a$ corresponds to the filtration coefficient of the soil.

3.3. The function $\theta$ (4) defines the water content in ZIS, and the derivative $\partial \theta / \partial t$ determines, on the one hand, the amount of water entering the soil through the earth surface, and on the other hand, – the velocity of the advancing front saturation in ZIS. The relationship (4) is obtained under the assumption that amount of water at the boundary of zone of incomplete saturation is enough to provide the maximum possible speed of its absorption. If the rainfall is less than they are completely absorbed by soil, and in this situation the volume of water incoming into ZIS should be determined not from the relation (4) but in a different way using the function $\varepsilon_i$:

Obviously, the velocity of the advancing front saturation will be decrease. Therefore, at $t > t_0$ when the intensity of rainfall will exceed the intensity of absorption and the water layer appears on the earth surface, the function $\partial \theta / \partial t$ becomes a function of the retarded argument $\tau_d$. In this case, it is required to define the values $t_0$ and $\tau_d$ for $\varepsilon_i > 2a$. Let $t_i = t_0 - \tau_d$. At the time point $t = t_0$ the intensity of rainfall is equal to the absorbtion intensity:
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\[
a^2 t_t + 0.5b \sqrt{a^2 t_t^2 + bt_t} + a = \varepsilon_1(t_0).
\]

(8)

By this time, the rainfall has completely been absorbed by soil in zone of incomplete saturation forming its water content. Hence we have:

\[
\sqrt{a^2 t_t^2 + bt_t} + at_t = A(t_0), \quad A(t_0) = \int_0^{t_0} \varepsilon_t d\tau.
\]

(9)

Solution to the system of nonlinear equations (8) and (9) can be obtained in terms of parameters \( t_0 \) and \( t_1 \). After their transformation we write the following expressions for \( t_0 \) and \( t_1 \):

\[
t_1 = \frac{b}{2a^2} \left( \frac{\varepsilon_1(t_0) - a}{\sqrt{\varepsilon_1^2(t_0) - 2ae_1(t_0)}} - 1 \right), \quad A(t_0) = \frac{b}{2a} \left( -1 + \frac{\varepsilon_1(t_0)}{\sqrt{\varepsilon_1^2(t_0) - 2ae_1(t_0)}} \right)
\]

(10)

The values of \( t_0 \) and \( t_1 \) are calculated from the equations (10), respectively. If at \( t < t_0 \) the function \( \varepsilon_1 \) is independent of time and \( \varepsilon_1 = \text{const} \) then \( a(t_0) = t_0 \varepsilon_1 \), so that the values of the lag time \( t_0 \) and the retarded argument \( \tau_d \) are defined as:

\[
t_0 = \frac{b}{2ae_1} \left( -1 + \frac{\varepsilon_1}{\sqrt{\varepsilon_1^2 - 2ae_1}} \right), \quad \tau_d = t_0 - t_1 = \frac{b}{2a^2} \left( 1 - \frac{a}{\varepsilon_1} - \sqrt{1 - \frac{2a}{\varepsilon_1}} \right)
\]

(11)

Thus, the surface runoff arises only at \( t = t_0 \) and the function \( \Theta \) for \( t > t_0 \) is calculated from the relationship with retarded argument:
\[
\Theta = \sqrt{a^2 (t - \tau_d)^2 + b(t - \tau_d) + a(t - \tau_d)}.
\]

3.4. The intensity of rainfall over time can become so insignificant that at an instant in time \( t_{cr} \) region \( D_{cr} \) with boundary \( \Gamma_{cr} \) will be formed where water completely soaks into the soil. In this case, the thickness of the surface water layer \( U(x, y, t) = 0 \) at \((x, y) \in D_{cr}, \ t > t_{cr}, \) and the water content in the soil is defined as:

\[
\Theta(x, y, t) = \Theta(x, y, t_{cr}) + \int_{t_{cr}}^{t} \varepsilon_i(x, y, \tau) d\tau.
\]

At those parts \( \Gamma^{-}_{cr} \) of the boundary \( \Gamma_{cr} \) where water flows out the region \( D_{cr} \), the function \( U \) is equal to zero and has no jumps. At the other parts \( \Gamma^{+}_{cr} \) this function can be discontinuous, and the water flow rate entering into the unsaturated zone is expressed as:

\[
\frac{\partial \Theta}{\partial t} = \varepsilon_i + V_n^+,
\]

where \( V_n^+ \) is the water flow through \( \Gamma^{+}_{cr} \). The area \( D_{cr} \) can vanish if the intensity of precipitation will increase. In this case, as in item 3, the values \( \bar{\tau}_d \) and \( \bar{\tau}_0 \) should be calculated at the instant of time when the intensity of rainfall exceeds the intensity of absorption, and the water layer appears on the earth surface. In this case \( \bar{\tau}_d \) and \( \bar{\tau}_0 \) are defined from the system that is similar to system (8), (9) and differs from these equations only in expression for \( A(t_0) \), namely:

\[
A(\bar{\tau}_0) = \Theta_{cr} + \int_{\bar{\tau}_0}^{\bar{\tau}} (\varepsilon_i + V_n^+) d\tau.
\]

3.5. At \( t < t_0 \) the surface-water flow is not formed \((U = 0)\), therefore \( C = 0 \), and in the area \( D_{cr} \) equation (3) allows for an analytical solution:

\[
C_s(x, y, t) = C_{s0}(x, y) e^{-\gamma t(1-m)} \approx C_{s0}(x, y) (1 - \gamma t / (1-m)).
\]

So, the problem is formulated as follows: we need to determine the solution \( U(x, y, t) \geq 0 \), \( \Theta(x, y, t) \), \( C(x, y, t) \) and \( C_s(x, y, t) \) of equations (1) – (4), (10) – (13)

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with initial and boundary conditions (5) and estimate the water flow rate in cross-section \( \Gamma_r \) of river at its lower course.

4. FINITE-DIFFERENCE SCHEME

The system of nonlinear differential equations for the runoff along the surface catchment and transfer of impurity coming into the stream from soil, is solved by the finite-difference methods proposed in (18). The initial region solution is subdivided into the unit cells of the grid \( D_h \) with the uniform step \( h_x \) and \( h_y \) along the axes \( Ox \) and \( Oy \) in such a way that the boundaries of cells were located at the boundary \( \Gamma \). Let us designate boundary of grid and the time step as \( \Gamma_h \) and \( \tau \).

It is typical of the surface runoff that \( |\nabla Z| \neq 0 \), and, as a rule \(|\nabla H| >> |\nabla U|\). Given the high uncertainty of the initial data let us assume in third and fourth equations (3) that \(|\nabla h| = |\nabla u|\). It would seem that the derivatives \( U'_x, U'_y \) can be ignored in these equations, and one assume that \( Z'_x = H'_x, Z'_y = H'_y \). However, at certain conditions \( U'_x, U'_y \) may have appreciable effects on the magnitude of the surface runoff. Therefore, the derivatives \( Z'_x, Z'_y \) in third and fourth equalities (6) can be approximately written in the following form \( Z'_x \approx \sqrt{H'_x + U'_x} \sqrt{H'_x}, Z'_y \approx \sqrt{H'_y + U'_y} \sqrt{H'_y} \). This allows to determine the values of these derivatives without error if the gradient \( \nabla Z = \nabla H \) is directed along the corresponding coordinate axis, i.e. at \( Z'_x = 0 \) or \( Z'_y = 0 \). Taking account of the characteristic features of the considered problem, we develop the implicit difference scheme consisting of linearized algebraic equations in which flows of water and of solution across the boundaries of the unit cells are approximated by the following relationship:

\[
\psi_{i,j} = \begin{cases} 
U'^{(r)}_{i+1/2,j}(U'^{(r)}_{i-1/2,j})^{2/3} V_{i+1/2,j}, & (x_{i+1/2,j}, y_j) \in D_h, \\
0, & (x_{i+1/2,j}, y_j) \in \Gamma_h 
\end{cases}
\]

(14)
\[
V_{i,j=1/2,2} = \begin{cases} 
\frac{h_z}{h_k} \text{sign}(Z_{i,z1,j} - Z_{i,j}) \sqrt{|Z_{i,z1,j} - Z_{i,j}|} \sqrt{H_{i,z1,j} - H_{i,j}}, \\
0, \\
(\chi, y_{j=1/2}) \in D_h,
\end{cases}
\]

(15)

\[
V_{i,j=1/2,1} = \frac{h_z}{h_k} \text{sign}(Z_{i,j=1} - Z_{i,j}) \sqrt{|Z_{i,j=1} - Z_{i,j}|} \sqrt{H_{i,j=1} - H_{i,j}},
\]

(16)

\[
K_{i,j=1/2} = \frac{\left( \frac{H_{i,j=1} - H_{i,j}}{2h_y} \right)^2 + \left( \frac{H_{i,j=1} - H_{i,j-1}}{2h_x} \right)^2 + \left( \frac{H_{i,j=1} - H_{i,j-1}}{2h_y} \right)^2}{\sqrt{\left( \frac{H_{i,j=1} - H_{i,j}}{2h_y} \right)^2 + \left( \frac{H_{i,j=1} - H_{i,j-1}}{2h_x} \right)^2}},
\]

It must be kept in mind that the real profile of the surface catchment can include topographical data at \( H_{i,j} < H_{i,j=1} \) and \( H_{i,j} < H_{i,j=1} \), so the gradient of inclination is directed along the diagonal of the unit cell, and liquid flows from the cell \( D_{i,j} \) into the one or even two cells adjoining to diagonal. In this case we need to determine not only the flows \( V_{i,j=1/2,2} \) and \( V_{i,j=1/2,1} \) but also the flows \( V_{i,j=1/2,2} \) from cell \( D_{i,j} \) into cells \( D_{i,j=1} \)
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and also \( \hat{W}_{i,j}^{\pm} \) from cell \( D_{i,j} \) into cells \( D_{i+1,j+1} \). To define these flows we introduce a new type of cells instead of the rectangular cells. Let \( H_{i,j} < H_{i+1,j} \) and \( H_{i+1,j+1} < H_{i,j+1} \) are satisfied then the main fluid flow is directed along the diagonal from cell \( D_{i,j} \) to the cell \( D_{i+1,j+1} \), and it is necessary to define the values of \( \hat{W}_{i+1/2,j} \) and \( \hat{W}_{i+1/2,j+1} \). It should be noted that if any one or more of these three conditions is not met, then \( \hat{W}_{i+1/2,j} = 0 \) and \( \hat{W}_{i+1/2,j+1} = 0 \). The modified cells \( D_{i,j}, D_{i+1,j}, D_{i,j+1} \) and \( D_{i+1,j+1} \) are shown in the Fig. 2.

![Fig. 2. Modification of cells in the case when the runoff is directed along the diagonal from the cell \( D_{i,j} \) to the cell \( D_{i+1,j} \).](image)

By the construction of these cells, the boundary \( M_1M_2 \) is orthogonal with the segments \( C_1D_1 \) and \( C_2D_2 \) which connect the midpoint of the respective sides of the rectangular cells. The length \( l \) of the segment \( M_1M_2 \) is equal to \( l = h_x h_y / \sqrt{h_x^2 + h_y^2} \), and the «diagonal» flows are determined by formulas:

\[
\hat{W}_{i+1/2,j} = U_{i,j}^{+\tau} \left( U_{i,j}^{-\tau} \right)^{2/3} \omega_{i+1/2,j}, \quad \hat{W}_{i+1/2,j+1} = \hat{W}_{i+1/2,j} C_{i,j}^{+\tau}.
\]

(17)

\[
\omega_{i+1/2,j} = -2l \sqrt{\left( Z_{i+1,j+1} - Z_{i,j} \right)} \left( n_{i,j} + n_{i+1,j+1} \right)^{-1} \left( h_x^2 + h_y^2 \right)^{-1/4}.
\]

Let us define the flows \( \nu_1, \nu_2, \nu_3 \) and \( \nu_4 \) through the boundaries \( A_1C_1M_1, M_1D_1B_1, A_2C_2M_2 \) and \( M_2D_2B_2 \), respectively. The components of these flows are defined from the relationships (14), (16) in segments \( A_1C_1, D_1B_1, A_2C_2 \) and \( D_2B_2 \), but in doing so, their magnitudes must become less by half due to decreasing of length of boundaries.
Consider now the other segments $C_i M_1$, $M_1 D_1$, $C_2 M_2$ and $M_2 D_2$. For $H_{i,j} > H_{i+1,j}$ the flow is directed from the cell $D_{i,j}$ into the cell $D_{i+1,j+1}$ through the cell $D_{i+1,j}$. We can assume that boundary $C_1 D_1$ goes along the stream-line and the normal flow velocity at this boundary is zero. Hence, the flows across the boundaries of $A_i C_i M_1$ and $M_1 D_1 B_1$ is equal to $0.5W_{i+1/2,j}$ and $0.5W_{i+1/2,j}$, respectively. If $H_{i,j} < H_{i+1,j}$ then the normal and tangent components $\theta_1$ and $\phi_1$ of the gradient surface inclination at $C_1 D_1$ can be approximated in the following form:

$$\theta_1 = \left[ \frac{h_x}{h_y} \left( H_{i+1,j} - H_{i,j} \right) + \frac{h_y}{h_x} \left( H_{i+1,j} - H_{i+1,j+1} \right) \right] \left( h_x^2 + h_y^2 \right)^{-1/2},$$

$$\phi_1 = \left[ H_{i+1,j+1} - H_{i,j} \right] \left( h_x^2 + h_y^2 \right)^{-1/2}.$$

Similarly, the approximations for the normal and tangent components $\theta_2$, $\phi_2$ of this gradient at the boundary $C_2 D_2$ for $H_{i,j} < H_{i,j+1}$ are:

$$\theta_2 = \left[ \frac{h_x}{h_y} \left( H_{i,j+1} - H_{i,j} \right) + \frac{h_y}{h_x} \left( H_{i,j+1} - H_{i+1,j+1} \right) \right] \left( h_x^2 + h_y^2 \right)^{-1/2},$$

$$\phi_2 = \phi_1.$$

Since the segments $C_1 M_1$, $C_2 M_2$ have the same length $l_1 = 0.5 h_i \sqrt{h_x^2 + h_y^2}$, and $M_1 D_1 = M_2 C_2 = l_2 = 0.5 h_i \sqrt{h_x^2 + h_y^2}$, the flow $\nu_1$, $\nu_2$, $\nu_3$, $\nu_4$ across the boundaries $A_i C_i M_i$, $M_1 D_1 B_1$, $A_2 C_2 M_2$, $M_2 D_2 B_2$ are determined by the relationships:

$$\nu_1 = U_{i+1,j}^{1/2} \left( U_{i+2,j}^{1/2} \right)^{2/3} \left( 0.5 V_{i+1/2,j}^{1/4} + l_1 \left( \theta_1^2 + \phi_1^2 \right)^{-1/4} \right),$$

$$\nu_2 = U_{i+1,j}^{1/2} \left( U_{i+2,j}^{1/2} \right)^{2/3} \left( 0.5 V_{i+1/2,j}^{1/4} + l_1 \left( \theta_1^2 + \phi_1^2 \right)^{-1/4} \right),$$

$$\nu_3 = U_{i,j+1}^{1/2} \left( U_{i,j+2}^{1/2} \right)^{2/3} \left( 0.5 V_{i+1/2,j}^{1/4} + l_1 \left( \theta_1^2 + \phi_1^2 \right)^{-1/4} \right),$$

$$\nu_4 = U_{i,j+1}^{1/2} \left( U_{i,j+2}^{1/2} \right)^{2/3} \left( 0.5 V_{i+1/2,j}^{1/4} + l_1 \left( \theta_1^2 + \phi_1^2 \right)^{-1/4} \right).$$

Thus, instead of the formulas (14) we have:
It is obvious that area of four modified unit cells are changed, namely,

\[ S_{i,j} = S_{i+1,j} = 9/8h_xh_y, \quad S_{i,j+1} = S_{i,j} = 7/8h_xh_y. \]

Note that if all the diagonal flows are equal to zero in the cell \( S_{i,j} \), then this cell doesn't change and its area is \( S_{i,j} = h_xh_y \). The values of other the «diagonal» flows \( \vec{V}_{i-1/2,j} \) and \( \vec{V}_{i,j+1/2} \) are determined in a similar way. It should be noted also that, given the great uncertainty of the input data, we can use more simple approximation for the flows across these boundaries, neglecting the second term in the brackets in (18), i.e. ignoring the flows across the boundaries \( C_iM_iD_i \) and \( C_2M_2D_2 \).

As is known, the derivatives in the convective terms of the transfer equations should be approximated by the upstream finite differences, using the values of the unknown function at the unit cell from which the liquid flows out:

\[
\frac{U_{i+1/2,j}^{t+\tau}}{U_{i-1/2,j}^{t}} = \begin{cases}
\frac{(U_{i+1/2,j}^{t+\tau})^2}{2/3}, & V_{i,j+1/2,j} \leq 0, \\
\frac{(U_{i-1/2,j}^{t+\tau})^2}{2/3}, & V_{i,j-1/2,j} < 0,
\end{cases}
\]

\[
\frac{U_{i,j+1/2}^{t+\tau}}{U_{i,j-1/2}^{t}} = \begin{cases}
\frac{(U_{i,j+1/2}^{t+\tau})^2}{2/3}, & V_{i+1,j+1/2} \leq 0, \\
\frac{(U_{i,j-1/2}^{t+\tau})^2}{2/3}, & V_{i-1,j+1/2} > 0,
\end{cases}
\]

\[
\frac{U_{i,j+2}^{t+\tau}}{U_{i,j-2}^{t}} = \begin{cases}
\frac{(U_{i,j+1}^{t+\tau})^2}{2/3}, & V_{i,j+1,j+2} < 0, \\
\frac{(U_{i,j-1}^{t+\tau})^2}{2/3}, & V_{i,j,j-1} \geq 0,
\end{cases}
\]
The conservative finite-difference scheme, approximating differential equations (1), (2) in the grid-points of the discrete domain $D_h$ can be written as:

$$\tau \Lambda \left[ \frac{\nabla Q_{i,j}}{\partial t} \right] = S_{i,j} \left( U_{i,j}^{t+\tau} - U_{i,j}^t - \Theta_{i,j}^{t+\tau} - \Theta_{i,j}^t - \tau \epsilon_{i,j} \right),$$

(20)

$$\epsilon_{i,j} = \frac{1}{\tau} \int \epsilon_j d\tau,$$

$$\tau \Lambda \left[ V_r + W_e \right]_{i,j} = S_{i,j} \left( C_{i,j}^{t+\tau} U_{i,j}^{t+\tau} - C_{i,j}^t U_{i,j}^t + \left( \Theta_{i,j}^{t+\tau} - \Theta_{i,j}^t \right) C_{i,j}^{t+\tau} - \tau \beta_{i,j}^{t+\tau} \right),$$

(21)

$$h \left( 1 - m \right) \left( C_{s,j,j}^{t+\tau} - C_{s,j,j}^t \right) = \tau \left( h \beta_{s,i,j}^{t+\tau} - \beta_{i,j}^{t+\tau} \right),$$

(22)

where $\Lambda \left[ \frac{\nabla Q_{i,j}}{\partial t} \right] = \frac{\epsilon_j}{\tau} \int d\tau$. It is convenient to rewrite the equations (21) and (22) in the following form:

$$C_{s,j,j}^{t+\tau} = C_{s,j,j}^t + b \left( C_{s,j,j}^t - C_{i,j}^{t+\tau} \right), \quad b = \frac{\tau \gamma}{1 - m + \tau \gamma},$$

(23)

$$C_{i,j}^{t+\tau} \left( U_{i,j}^{t+\tau} - \Theta_{i,j}^{t+\tau} + \tau \alpha \lambda \right) - C_{i,j}^t U_{i,j}^t - \tau \alpha \lambda C_{i,j}^{t+\tau} = \tau \Lambda \left[ V_r + W_e \right]_{i,j} / S_{i,j}^t,$$

(24)

$$d = \frac{1 - m}{1 - m + \tau \left( \gamma + \lambda / \lambda h \right)}.$$
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value over the area and time. Therefore, the lag time $t_0$ and the retarded argument $\tau_{d,i,j}$ can be obtained from equalities (11) at $\varepsilon_i > 2a$.

If parameters $a$, $b$ and $\varepsilon_i$ in Eq. (11) are functions of the coordinates $(x, y)$ then the values of $t_0$ and $\tau_d$ depend on the mesh node $(x_i, y_j)$. In this case a minimum value $\bar{t}_0 = \min_{D_{i,j}} t_0(x_i, y_j)$ is defined, and from this point on it is assumed by the new initial moment in computation. Obviously, $\bar{t}_0 = 0$ if $a = b = 0$ in some mesh nodes (e.g., if they located in the river bed). In those unit cells where the lag time is greater than $\bar{t}_0$, it is required to recalculate the values of $\bar{t}_0$ with account for possible inflows from the surrounding cells. Actually, in computation with the use of the implicit scheme already at the first point of time $\bar{t}_0 + \tau$, the flows of water arise across the boundaries of neighboring grid cells in which $t_0 > \bar{t}_0$. Let, for example, $t_0 > \bar{t}_0$ in the unit cell $D_{i,j}$ and water enters into it from the surrounding cells. Hereinafter, we denote the total amount of all flows coming into the grid cell as $w^+$, and the intensity of water inflow into the cell at $t_0 > \bar{t}_0$ as $\varepsilon_w = w^+ + \varepsilon_{1,i,j}$. Since at $t_0 < \bar{t}_0$ water, inflowing into the unit cell $D_{i,j}$, is completely absorbed by the soil of ZIS, so the water amount $A(t_0)$ in this zone at time $t_0$ is defined as: $A(t_0) = A(\bar{t}_0) + (t_0 - \bar{t}_0)\varepsilon_w$, where $A(\bar{t}_0)$ is amount of water in ZIS at $t = \bar{t}_0$. In this case $A(\bar{t}_0) = \int_0^{\bar{t}_0} \varepsilon_{1,i,j} dt$. Thus, the new values $t_0$ and $\tau_d$ are determined from the same system equations (8) and (9), but with other right-hand parts. The solution of this system is:

$$t_0 = \bar{t}_0 + \frac{b}{2a\varepsilon_w} \left( \frac{1}{\sqrt{1 - 2a/\varepsilon_w}} - 1 \right) \frac{A(\bar{t}_0)}{\varepsilon_w}.$$  (25)

If $t_0 - \bar{t}_0 < \tau$ then the retarded argument $\tau_{d,i,j}$ is calculated from formula
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\[ \tau_{d,i,j} = \bar{\tau}_{0} + \frac{b}{2d^2} \left( 1 - \frac{a}{\varepsilon_w} - \sqrt{1 - 2a/\varepsilon_w} \right) \frac{A(\bar{\tau}_{0})}{\varepsilon_w} \]

(26)

and the water content \( \Theta_{i,j}^{\star \tau} \) in zone of incomplete saturation is defined by equality (12) at \( \tau_d = \tau_{d,i,j} \). The thickness \( U_{i,j}^{\star \tau} \) of water layer is calculated from the algebraic equation (20) for discrete time \( \bar{\tau} = \tau - (t_0 - \bar{\tau}_0) \).

If \( t_0 > \bar{\tau}_0 + \tau \) then the above procedure computation of values \( t_0 \) and \( \tau_{d,i,j} \) is similarly repeated in the next time point.

In much the same way as reported previously the problem is solved at formation of such regions on the surface catchment in which the water layer temporarily disappears in result of its absorbtion by soil. Let \( \Theta_{i,j}^{\star \tau} \) be the water amount in ZIS, calculated from formula (12). Then from the inequality

\[ \tau w^* / S_{i,j} + U_{i,j} - \Theta_{i,j}^{\star \tau} + \Theta_{i,j} + \tau w_{i,j} < 0 \]

it follows that at \( U_{i,j} > 0 \) the rainwater is completely adsorbed and \( U_{i,j} = 0 \). Therefore, \( \Theta_{i,j}^{\star \tau} \) should be calculated not from formula (12) but from equation

\[ \Theta_{i,j}^{\star \tau} = U_{i,j} + \Theta_{i,j} + \tau w_{i,j} + w^* / S_{i,j} \]

(27)

If \( U_{i,j} = 0 \) then the lag time \( t_0 \) is defined from formula (25) at \( A(\bar{\tau}_0) = \Theta_{i,j} \) and, if it is necessary the values \( \tau_{d,i,j} \) are also recomputed from relationship (26). As well as we do earlier, at \( t_0 - \bar{\tau}_0 < \tau \) the retarded argument \( \tau_{d,i,j} \) is computed from formula (26), the amount of water \( \Theta_{i,j}^{\star \tau} \) in ZIS – in accordance with equality (12) for the current value of \( \tau_{d,i,j} \), and the thickness of the water layer \( U_{i,j}^{\star \tau} \) – from the difference equations (20) at the time point \( \bar{\tau} = \tau - (t_0 - \bar{\tau}_0) \). At \( t_0 > \bar{\tau}_0 \) the thickness \( U_{i,j}^{\star \tau} = 0 \), the mesh function...
\( \Theta_{i,j}^{\tau+\vartheta} \) is defined from formula (27), and the values of \( t_0 \) and \( \tau_{d,i,j} \) are calculated all over again at the next point in time.

With the appearance of region \( D_{cr} \) with vanishing water layer the concentration of contaminant becomes equal to zero: \( C_{i,j}^{\tau+\vartheta} = 0 \). However, the impurity can flow into the grid cells located at the boundary \( \Gamma_{cr} \) of this region from the adjacent unit cells. This contaminant is completely absorbed by soil of ZIS. Let us denote the total quantity of all the incoming flows with the impurity into the cell \( D_{i,j} \) as \( w_{i}^* \), and the impurity concentration of in the water solution which enters into the zone of incomplete saturation over time \( \tau \) as \( \overline{C} \). Now we can write the following relationship for \( \overline{C} \):

\[
\overline{C} = \left( C_{i,j} U_{i,j} + \tau w_{i}^* / S_{i,j} \right) / \left( \Theta_{i,j}^{\tau+\vartheta} - \Theta_{i,j} \right),
\]

where \( \Theta_{i,j}^{\tau+\vartheta} - \Theta_{i,j} \) is calculated from equation (27). Then the function \( C_{s,i,j}^{\tau+\vartheta} \) is defined as:

\[
C_{s,i,j}^{\tau+\vartheta} = C_{s,i,j}^\tau - \frac{\tau \gamma}{1 - m + \tau \gamma} \left( C_{s,i,j}^\tau - \overline{C} \right).
\] (28)

5. COMPUTATIONAL ALGORITHM

Difference scheme (14)–(28) consists of two systems of linear algebraic equations. The first of them is obtained in result of linearization of the implicit difference scheme in respect to the functions \( U \) and does not depend on concentration \( C \). The second one is used to determine of \( C \) from system of linear equations after computation of \( U \). Both systems can be transformed to diagonal form by renumbering the grid cells in a different way: either in descending order of \( Z \) or of \( H \). This allows us to solve equations sequentially starting with the first equation corresponding to the maximum height of the catchment relief.

The first procedure requires the transformation of the system matrix at every time point. The second approach allows us to do such transformation only once in the beginning of the problem solution, that significantly reduces the calculations required and overall computation time. However, in those situations when \( (H_{i+1,j} - H_{i,j})(Z_{i+1,j} - Z_{i,j}) < 0 \), the...
runoff can goes upslope (e.g. at flooding of the river banks during the period of overflow), so that the coefficient matrix of a system of linear algebraic equations loses its diagonal form. To avoid this, we impose an additional conditions on

\[ U_{i,j}^{t\rightarrow\tau}(U_{i,j}^{t\rightarrow\tau})^{2/3}, U_{i,j+1/2}^{t\rightarrow\tau}(U_{i,j+1/2}^{t\rightarrow\tau})^{2/3}, C_{i,j+1/2}^{t\rightarrow\tau}, C_{i+1/2,j}^{t\rightarrow\tau} \] in the relationships (19):

\[
U_{i,j}^{t\rightarrow\tau}(U_{i,j}^{t\rightarrow\tau})^{2/3} = \begin{cases} 
U_{i,j}^{t\rightarrow\tau}, & V_{i,j} < H_{i,j}, \\
U_{i,j}^{t\rightarrow\tau}(U_{i,j}^{t\rightarrow\tau})^{2/3}, & V_{i,j} > H_{i,j}, \\
U_{i,j}^{t\rightarrow\tau}(U_{i,j}^{t\rightarrow\tau})^{2/3}, & V_{i,j} > H_{i,j},
\end{cases}
\]

\[
U_{i,j+1/2}^{t\rightarrow\tau}(U_{i,j+1/2}^{t\rightarrow\tau})^{2/3} = \begin{cases} 
U_{i,j+1/2}^{t\rightarrow\tau}, & V_{i,j+1/2} < 0, \\
U_{i,j+1/2}^{t\rightarrow\tau}(U_{i,j+1/2}^{t\rightarrow\tau})^{2/3}, & V_{i,j+1/2} > 0, \\
U_{i,j+1/2}^{t\rightarrow\tau}(U_{i,j+1/2}^{t\rightarrow\tau})^{2/3}, & V_{i,j+1/2} > 0,
\end{cases}
\]

\[
U_{i,j+1/2}^{t\rightarrow\tau}(U_{i,j+1/2}^{t\rightarrow\tau})^{2/3} = \begin{cases} 
U_{i,j+1/2}^{t\rightarrow\tau}, & V_{i,j+1/2} > 0, \\
U_{i,j+1/2}^{t\rightarrow\tau}(U_{i,j+1/2}^{t\rightarrow\tau})^{2/3}, & V_{i,j+1/2} > 0, \\
U_{i,j+1/2}^{t\rightarrow\tau}(U_{i,j+1/2}^{t\rightarrow\tau})^{2/3}, & V_{i,j+1/2} > 0,
\end{cases}
\]

\[
U_{i,j-1/2}^{t\rightarrow\tau}(U_{i,j-1/2}^{t\rightarrow\tau})^{2/3} = \begin{cases} 
U_{i,j-1/2}^{t\rightarrow\tau}, & V_{i,j-1/2} < 0, \\
U_{i,j-1/2}^{t\rightarrow\tau}(U_{i,j-1/2}^{t\rightarrow\tau})^{2/3}, & V_{i,j-1/2} > 0, \\
U_{i,j-1/2}^{t\rightarrow\tau}(U_{i,j-1/2}^{t\rightarrow\tau})^{2/3}, & V_{i,j-1/2} > 0,
\end{cases}
\]

\[
C_{i,j}^{t\rightarrow\tau} = \begin{cases} 
C_{i,j}^{t\rightarrow\tau}, & V_{i,j} < H_{i,j}, \\
C_{i,j}^{t\rightarrow\tau}, & V_{i,j} > H_{i,j}, \\
C_{i,j}^{t\rightarrow\tau}, & V_{i,j} > H_{i,j},
\end{cases}
\]

\[
C_{i+1/2,j}^{t\rightarrow\tau} = \begin{cases} 
C_{i+1/2,j}^{t\rightarrow\tau}, & V_{i,j+1/2} < 0, \\
C_{i+1/2,j}^{t\rightarrow\tau}, & V_{i,j+1/2} > 0, \\
C_{i+1/2,j}^{t\rightarrow\tau}, & V_{i,j+1/2} > 0,
\end{cases}
\]

\[
C_{i-1/2,j}^{t\rightarrow\tau} = \begin{cases} 
C_{i-1/2,j}^{t\rightarrow\tau}, & V_{i,j-1/2} < 0, \\
C_{i-1/2,j}^{t\rightarrow\tau}, & V_{i,j-1/2} > 0, \\
C_{i-1/2,j}^{t\rightarrow\tau}, & V_{i,j-1/2} > 0,
\end{cases}
\]
The computational algorithm is the following. Let the values of the difference functions $U_{i,j}^t$, $\Theta_{i,j}^t$, $C_{i,j}^t$ and $C_{s,i,j}^t$ are determined in the mesh nodes $(x_i, y_j)$ at the time point $t$.

With these values the flows $V_{i,j+1/2}^t$, $V_{i,j-1/2}^t$, $\omega_{i+1/2,j}^t$, $\omega_{i,j+1/2}^t$ and the water flow rate of river through its cross-section $\Gamma_r$ are calculated at the boundaries of unit cells from relationships (14), (16). Then, starting with the first cell, we calculate the water amount $\Theta_{i,j}^{t+\tau}$ in zone of incomplete saturation, the thickness $U_{i,j}^{t+\tau}$ of the water layer on the catchment surface and the values of the fluid flows going out from the unit cells. If $U_{i,j}^t = 0$, then the lag time $\tau_0$ and the retarded argument $\tau_d$ are additionally computed.

The total amount of water crossing the boundary $\Gamma_r$ is determined as sum of the corresponding flow-rates with time in the nodes of the shifted grid located at $\Gamma_r$. After this the flows $V_{c,i+1/2,j}^t$, $V_{c,i-1/2,j}^t$ and $W_{c,i,j+1/2}^t$, $W_{c,i,j-1/2}^t$ are calculated from (15), (17). At last, the impurity concentration $C_{i,j}^{t+\tau}$ in the rainwater runoff is determined from the system equations (24) and the contaminant concentration $C_{s,i,j}^{t+\tau}$ in fluid moving in the soil – from the formulas (23).

Solution of a problem at the time point $t + \tau$ is finished after the calculation of disbalances to check the computation accuracy, data preparation for computation at next time point and checking the condition of the end of simulation.

The developed numerical model and solution algorithms were implemented in the program package SURFLOW-C to simulate the rainwater runoff along with simultaneous graphic visualization of the computational results.
6. SUMMARY

The main theoretical results of this work can be briefly formulated as following.
1. The mathematical model of runoff along the surface catchment taking account precipitation, evaporation, transport of impurity in water, its filtration in zone of incomplete saturation of soil, sorption and adsorption of pollutant in soil is proposed.
2. The principal features of the problem solution are theoretically studied.
3. The finite-difference scheme and the corresponding software to solve the system of nonlinear differential equations are developed using a priori information about the solution behavior and the modified grid cells for computation of «the diagonal flows» between the neighbor cells.

The features of the water runoff and the impurity migration in the river basin will be investigated with the use of natural data and presented in our future publications.

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8. BIBLIOGRAPHY


