Models of dynamics of contamination propagation in surface waters using simulation of hydrodynamical processes of different level of complexity.

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Abstract. This paper uses the ideology of solving hyperbolic equations using the Euler balance-characteristic approach, which allows economically and correctly resolving the dynamics of pollution propagation processes with large concentration gradients characteristic of an accident. The purpose of the study is to develop a three-dimensional model of advection-diffusion in a non-uniform velocity field and non-isotropic field of turbulent diffusion, taking into account some physical processes: gravity sedimentation, sediment accumulation and their dynamics. As well as the implementation of the interaction model with the hydrodynamic module, based on solving the equations of the theory of shallow water in the approximation of Saint-Venant.

1. The equations of advection-diffusion and deformation of the bottom
Consider the advection-diffusion equation in differential form for the impurity:

\[
\frac{\partial C}{\partial t} + \frac{\partial UC}{\partial x} + \frac{\partial VC}{\partial y} + \frac{\partial(W - w_g)C}{\partial z} = \nabla (\nu \cdot \nabla C) - q_{sed}
\]  

(1)

where \( C \) - is the concentration of radionuclides; \( U, V, W \) - components of the flow velocity, \( w_g \) - gravitational speed of sedimentation of suspended particles; \( \nu \) - is the coefficient of turbulent diffusion, \( q_{sed} \) - is the flow of particles to the bottom. Equation (1) is also valid for the dissolved form of radionuclides with \( w_g = 0 \) \( q_{sed} = 0 \).

Together with (1), we also consider the one-dimensional bottom deformation equation:

\[
\rho_s (1 - \varepsilon) \frac{\partial Z}{\partial t} + \frac{\partial p_{tr}}{\partial x} = Q_{in}
\]  

(2)

where \( Z \) - is the height of sedimentation of the impurity, \( \rho_s \) - is the density of particles, \( \varepsilon \) - is the porosity of sediments, \( p_{tr} \) is the elementary consumption of traction sediment \( \frac{k_g}{m/s} \), \( Q_{in} \) - is the source term.

In turn, the flow of sediment load is proposed to be approximated by the formula proposed by I.I. Levi [2]:

\[
p_{tr} = k_0 \left( \frac{u(x)}{\sqrt{gd}} \right)^3 \left( u(x) - u_{beg} \right) \left( \frac{d}{L_z - Z(x)} \right)^{0.25}
\]  

(3)
where \(k_0\) is a parameter, \(u(x)\) is the flow velocity above the bottom, \(d\) is the average particle diameter, \(g\) is the acceleration of gravity, \(v_{beg}\) is the average flow velocity at which particles are captured by the flow and start moving, \(L_z - Z(x)\) is the depth flow. In [2], expressions for the calculation at the beginning velocity are also given, for example, the formula of V.N. Goncharov. In this paper, the specification of formulas is not so important, in all the calculations performed, the beginning velocity is constant. Let us consider the problem of sedimentation of suspended particles in a uniform flow under boundary conditions of free flow on the walls of the region, total reflection at the upper boundary and the condition of complete absorption at the lower boundary. Deposition occurs from the bottom settlement cells; \(q_{sed}\) is zero everywhere except \(z = 0\). Based on this, we arrive at the equation:

\[
\rho_s (1 - \varepsilon) \frac{\partial Z}{\partial t} + \frac{\partial p_{tr}}{\partial x} = \frac{1}{h_z} \left( \nu \frac{\partial C_{bot}}{\partial z} + w_g C_{bot} \right)
\]

(4)

where \(C_{bot}\) is the impurity concentration at the bottom, \(h_z\) is the height of the computational cell. The first term on the right (4) is the diffusion flow of particles due to the condition of complete absorption, and the second is the advective flow caused by the vertical movement of particles under the action of gravity.

The vertical derivative of the concentration of suspension in the bottom cell, taking into account the condition of complete absorption will be approximately equal to:

\[
\left. \frac{\partial C_{bot}}{\partial z} \right|_{z=0} = \frac{C_{bot} - 0}{h_z/2} = \frac{2C_{bot}}{h_z}
\]

(5)

Because of the law of conservation of mass:

\[
q_{sed}|_{z=0} = \frac{\partial C_{bot}}{\partial t} = - \frac{1}{h_z} \left( \nu \frac{\partial C_{bot}}{\partial z} + w_g C_{bot} \right) = - \frac{1}{h_z} \left( \nu \frac{2C_{bot}}{h_z} + w_g C_{bot} \right)
\]

(6)

For the time step, the average concentration in the bottom cell due to precipitation processes will change as follows:

\[
C_{bot} (t + \tau) = C_{bot} (t) \exp \left\{ -\tau \left( \frac{2\nu_z}{h_z^2} + \frac{w_g}{h_z} \right) \right\}
\]

(7)

If we divide the deformation equation (4)

\[
\rho_s (1 - \varepsilon) \frac{\partial Z}{\partial t} + \frac{\partial p_{tr}}{\partial x} = \frac{1}{h_z} \left( \nu \frac{\partial C_{bot}}{\partial z} + w_g C_{bot} \right)
\]

(8)

\[
\rho_s (1 - \varepsilon) \frac{\partial Z}{\partial t} + \frac{\partial p_{tr}}{\partial x} = 0
\]

(9)

That level of bottom sediments according to the equation (8) will change as follows:

\[
Z (t + \tau) = Z (t) + \frac{C_{bot} (t) h_z}{\rho_s (1 - \varepsilon)} \left[ 1 - \exp \left\{ \tau \left( \frac{2\nu_z}{h_z^2} + \frac{w_g}{h_z} \right) \right\} \right]
\]

(10)

And the equation (9) is calculated according to the CABARE method in the next paragraph of the paper.
2. CABARE scheme for the nonlinear bottom deformation equation

Simplify the representation of the equation (9) to the form:

$$\frac{\partial Z}{\partial t} + \frac{\partial p}{\partial x} = 0$$  \hspace{1cm} (11)

Before proceeding with the calculation, the initial agreement of the conservative and flow variables is performed in the following procedure:

$$Z^0_i = \frac{1}{2} \left( Z^0_{i-1/2} + Z^0_{i+1/2} \right)$$  \hspace{1cm} (12)

Fractional indices correspond to the centers of the calculated cells. Integer indices correspond to boundaries.

In the first phase, the calculation of conservative variables on the half-integral layer takes place:

$$\frac{Z_{i+1/2}^n - Z_{i+1/2}^n}{\tau/2} + \frac{p_{i+1}^n - p_i^n}{x_{i+1} - x_i} = Q$$  \hspace{1cm} (13)

In this equation, $Q = 0$ is the term approximating the source and diffusion. Thus, the values of heights are calculated through time $\tau/2$ in the centers of the calculated cells. In the next step, the initial values of heights are calculated through time at the boundaries of the calculated cells, that is, the flow variables:

$$\tilde{Z}_{i+1}^n = \begin{cases} 2Z_{i-1/2}^n - Z_{i-1}^n, U > 0; & Z_i^n, U = 0; \ 2Z_{i+1/2}^n - Z_{i+1}^n, U < 0. \end{cases}$$  \hspace{1cm} (14)

Where $U = \frac{\partial p}{\partial Z}$ is nominal transfer rate in the equation.

Then differentiating the expression (11) by the $x$ coordinate and substituting (3):

$$\frac{\partial p}{\partial x} = U \frac{\partial z}{\partial x} = \frac{1}{2} \frac{u^3 (u - v_{beg})}{4 \rho_s (1 - \varepsilon)h_x g^3/2D_{5/4}(L_z - Z(x))^5/4} \frac{\partial z}{\partial x}$$  \hspace{1cm} (15)

Here we consider $u$ to be a constant independent of coordinates. The limit on the time step is determined by the Courant expression:

$$\tau < CFL \cdot \frac{h_x}{U}; \tau < \frac{1}{2} \cdot \frac{h_x}{\max(U)}$$  \hspace{1cm} (16)

Where $CFL = \frac{1}{2}$ is Courant number. Next, a nonlinear correction of flow variables is performed.

$$Z_i^{n+1} = \text{MIN} \left( \text{MAX} \left( \tilde{Z}_i^{n+1}, Z_{\text{min}} \right), Z_{\text{max}} \right)$$  \hspace{1cm} (17)

In these equations, $Z_{\text{min}}$ and $Z_{\text{max}}$ is the estimate of the maximum and minimum height of the impurity at the time layer $n + 1$ in the cell from which the extrapolation was made, which depends on the direction of the flow velocity. At the next stage, the concentrations in the centers of the cells on the $n + 1$ layer are calculated:

$$\frac{Z_{i+1/2}^{n+1} - Z_{i+1/2}^n}{\tau/2} + \frac{p_{i+1}^{n+1} - p_i^{n+1}}{x_{i+1} - x_i} = Q_{i+1/2}^{n+1}$$  \hspace{1cm} (18)

The right side is zero in this case. This completes the method step.
3. Model problems of rupture

3.1. Discharge Wave

The initial gap cannot be infinite. It is defined as a linear function with a large slope. To find a solution to equation (15), an integral method was used to find the exact solution. Each point of the profile $X(z)$ moves with speed:

$$U = \frac{1}{4} \frac{u^3(u-v_{beg})}{\rho_s(1-\varepsilon)h_x g^{3/2}d^{5/4}(L_z-Z(x))^{5/4}} = \frac{ac}{(L_z-Z(x))^{a+\frac{4}{5}}}. \tag{19}$$

In this way

$$X^{n+1}(z) = X^n(z) + U \cdot \tau \tag{20}$$

The solution obtained by this method will be indicated on the graphs by a red line, and the solution obtained by the CABARE method will be indicated by blue triangular points. Below are the results of the calculation at nominal time points of 200 and 500 s for a problem with the following initial conditions in nominal values.

$$Z_0 = \begin{cases} 100, & \text{if} \ x > \delta; \\ \frac{50}{\delta} x + 50, & \text{if} \ x \in [0, \delta]; \\ 50, & \text{if} \ x < 0 \end{cases} \tag{21}$$

where $\delta = 1.$

![Figure 1. Initial distribution](image1)

**Figure 1.** Initial distribution

![Figure 2. Result of the calculation at 200 s](image2)

**Figure 2.** Result of the calculation at 200 s

![Figure 3. Result of the calculation at 500 s](image3)

**Figure 3.** Result of the calculation at 500 s
3.2. Shock wave

We represent equation (11) in a divergent form:

$$\int_G \left( \frac{\partial p}{\partial x} + \frac{\partial Z}{\partial t} \right) dx dt = \oint \frac{Z dx}{\partial G} - p dt = 0$$

(22)

$$(Z_R - Z_L) \Delta x - (p_R - p_L) \Delta t = 0$$

(23)

$$V_{gap} = \frac{\Delta x}{\Delta t} = \frac{p_R - p_L}{Z_R - Z_L} = \frac{c}{Z_R - Z_L} \left( \frac{1}{(Z_L - Z_R)^a} - \frac{1}{(Z_L - Z_L)^a} \right)$$

(24)

Expression (24) represents the velocity of the gap.

Below are the results of the calculation at nominal time points of 150 and 450 s for a problem with the following initial conditions in nominal values.

$$Z_0 = \begin{cases} 50, & i f x > \delta; \\ 100 - \frac{50}{\delta} x, & i f x \subset [0, \delta]; \\ 100, & i f x < 0 \end{cases}$$

where $\delta = 1$.

Figure 4. Result of the calculation at 150 s

Figure 5. Result of the calculation at 450 s

3.3. The task of precipitation of impurities on the bottom, taking into account the dynamics

Consider the complex problem of advection-diffusion of impurities in the aquatic environment and the deformation of bottom sediments. We take the initial distribution of concentrations in the form of three homogeneous strips of different shapes at different distances from each other. Let be

$$C_0 = \begin{cases} 1, & i f x \subset [x_1, x_2] \bigcup [x_3, x_4] \bigcup [x_5, x_6]; \\ 0, & e l s e \end{cases}$$

(26)

$$Z_0(x) = 0$$

(27)
Figure 6. Initial concentration profile

Figure 7. Initial profile of deposition heights

Figure 8. Result of the calculation at 10 s

Figure 9. Result of the calculation at 10 s

Figure 10. Result of the calculation at 40 s

Figure 11. Result of the calculation at 40 s

Figure 12. Result of the calculation at 100 s

Figure 13. Result of the calculation at 100 s

References

[1] Goloviznin V.M., Zaitsev M.A., Karabasov S.A., Korotkin I.A. 2013 New Algorithms of Computational Fluid Dynamics (Moscow: Moscow State University Press)

[2] A.V. Karaushev 1977 Theory and Methods for the Calculation of River Sediments (Publishing House - Gidrometeoizdat)