Dispersion of conservative impurities in rivers: implications for compliance with environmental standards

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Abstract. The research goal is to understand the mechanisms of transport and transformation of conservative impurities in river flows and provide practical solutions to ensure compliance with environmental standards. The need to close the system of equations and make it suitable for solving practical problems caused the addition of equations of motion with empirical regularities. We use an approach based on fundamental equations of hydrodynamics. The main task of mathematical transformations of the fundamental equations was: a) considering the variability of the turbulent exchange coefficients along the flow cross-section. b) addition of the obtained equations with empirical regularities linking the flow characteristics with the turbulent exchange coefficients. c) mathematical transformations were performed to obtain a group of closed equations for which approximate solution methods are known and developed. The best empirical regularities in determining the turbulent exchange coefficients were selected by applying a closed mathematical model. For each desired variable, we obtained an equation of the evolutionary type, which lends itself well to algorithmization. The schemes presented in the article allow us to design computational algorithms using classical approaches to solving impurity transfer equations with variable coefficients of turbulent exchange.

1 Introduction

Rivers are vital components of many ecosystems, providing habitat for diverse communities of plant and animal life and serving as sources of drinking water, irrigation, and recreation for human populations. However, rivers are also vulnerable to pollution from various sources, including industrial and agricultural activities, urbanization, and transportation [1,2]. While some types of pollutants can be readily removed or treated, others, known as conservative impurities, persist in the water and can be transported over long distances, potentially causing harm to ecosystems and human health [3–5].

To understand and manage the risks posed by conservative impurities in rivers, studying their transport and fate under different environmental conditions is necessary. This involves

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investigating the impact of factors such as flow rate, sunlight, water temperature, and the presence of life forms on the mixing and dispersion of conservative impurities in the water. It also requires developing mathematical models that can accurately predict the behavior of these impurities and evaluating the effectiveness of different remediation strategies [6–9].

In this context, many potential research questions could be explored. These might include investigating the optimal discharge regimes for different types of conservative impurities, evaluating the effectiveness of different remediation strategies, and developing new measurement techniques to improve our understanding of the transport and fate of these impurities in rivers. Ultimately, this research aims to develop strategies for managing conservative impurities in rivers that balance economic development with environmental protection and to ensure the long-term sustainability of these important ecosystems.

Study area. The territory of the research object covers the Beruni, Turtkul, and Ellikkala districts of Southern Karakalpakstan, with a total area of about 1000 sq km. Channels with water intake from the Amu Darya River, the Tuyamuyun reservoir, and the Drainage system connected to the Main South Karakalpak collector are located on this territory.

2 Materials and methods

When moving along the river, the impurity entering the stream is pointwise mixing and spreading of the impurity throughout the river stream [10–12].

Suppose the admixture is conservative (mineralization) and the inflow of admixture into the river is constant. In that case, the total admixture flux through the cross-section of the riverbed does not change. If the admixture is not conservative (COD, BOD) and the influx of admixture into the river is constant, then the total admixture flux through the cross-section of the river channel may change [13,14].

Special studies are required to calculate changes in the concentration of non-conservative impurities with a huge number of individual high-precision specialized measurements and observations. It is unlikely that there is any specific universal set of research activities or measurements applicable to all rivers. Each case will be unique. Each case will depend on the life forms peculiar to the watercourse. Each case will depend on the set of chemical elements already present in the river. Water transparency, sunlight, water temperature, and turbulence of flowing water will play a role. In this regard, the only practically acceptable solution should be the desire to reach the same COD and BOD values in the river below the discharge point, observed before impurities' discharge into the river [15–20]. But to find this solution, considerable time and considerable effort from a variety of highly qualified specialists are required. A huge number of field measurements are required. And even in this case, the result will be approximate due to the particular complexity of the problem being solved. One mathematical modeling without a complex of full-scale measurements cannot cope with the task. Therefore, in the framework of this work, the transformation of the spot of non-conservative impurities will not be considered.

The motion and transformation of a conservative impurity spot can be calculated quite accurately. It is even possible to find such regimes for the discharge of impurities into the river (depending on the water flow in the river) that will ensure the fulfillment of environmental requirements for compliance with environmental standards [21–23].

The basis for calculating the movement and transformation of impurities will be the equation of motion of water in the river (two-dimensional, horizontal) and the equation of conservation of the mass of conservative impurities[24].

3 Results and Discussion

When calculating the transformation of spots of impurities entering the river, the equations of Saint-Venant are usually used to calculate water velocities [25–29]

$$\frac{\partial h}{\partial t}+\frac{1}{b}\cdot\frac{\partial Q}{\partial x}$$

$$\frac{1}{g}\cdot\frac{\partial \mathcal{U}}{\partial t}+\frac{\mathcal{U}}{g}\cdot\frac{\partial \mathcal{U}}{\partial x}+\frac{\partial h}{\partial x}-J+\frac{Q^2}{K^2}=0 \quad (1)$$

And the admixture conservation equation

$$\frac{\partial S}{\partial t}+\frac{\partial(S\cdot \mathcal{U})}{\partial x}=+\frac{\partial D_s \partial S}{(\partial x)^2}+\mathrm{I} \quad (2)$$

where
h is flow depth, meter,
∂ is sign of the derivative, b.r.,
t is time, sec,
b is flow width, meter,
Q is water flow, $\frac{\mathrm{meter}^3}{sec}$,
x is distance along the river, meter,
g is free fall acceleration, $\frac{meter}{sec^2}$,
$\mathcal{U}$ is speed of water movement, $\frac{meter}{sec}$,
J is slope of the bottom of the riverbed, b.r.,
K is coefficient of friction, $\frac{meter^3}{sec}$,
S is impurity concentration, $\frac{kg}{meter^3}$,
D_s is diffusion coefficient, $\frac{meter^2}{sec}$,
I is point source of impurity, $\frac{kg}{meter^3 \cdot sec}$.

The average pollution of any cross-section of the river is not very informative. In our cases, this is not enough. The next important water intake from the river in the densely populated area of the middle reaches of the Akhangaran, Chirchik, and Syrdarya rivers near Bekabad may be at the center of an unacceptable concentration of a pollution spot. However, the average situation may seem quite optimistic over the river cross-section [30].

For us, the spatial distribution of the spot of impurities along the river is important. The calculation of the three-dimensional propagation of a conservative impurity is certainly possible. However, the expected efforts in solving the three-dimensional problem significantly exceed the small increase in the information content of the result, which can be obtained by considering the vertical component in the transformation of the impurity spot. Therefore, the equation of impurity conservation integrated along the vertical from the bottom position point to the free surface point will be used for the calculation.

$$\frac{\partial S}{\partial t}+\frac{\partial(S\cdot V)}{\partial x}+\frac{\partial(S\cdot U)}{\partial y}=+\frac{\partial D_s \partial S}{(\partial x)^2}+\frac{\partial D_s \partial S}{(\partial y)^2}+\mathrm{I}$$

$$\frac{\partial V}{\partial t}+V\frac{\partial(V)}{\partial x}+U\frac{\partial(V)}{\partial y}=+\frac{\partial h_p}{\rho\cdot\partial x}+\frac{\partial D_v \partial V}{(\partial x)^2}+\frac{\partial D_v \partial V}{(\partial y)^2}+K_z\cdot\frac{V}{h^2} \quad (3)$$

$$\frac{\partial U}{\partial t}+ V\frac{\partial(U)}{\partial x}+U\frac{\partial(U)}{\partial y}=+\frac{\partial h_p}{\rho\cdot\partial y}+\frac{\partial D_v \partial U}{(\partial x)^2}+\frac{\partial D_v \partial U}{(\partial y)^2}+K_z\cdot\frac{U}{h^2}$$

$$\frac{\partial h_p}{\partial t}=\int_{z=o}^{x=h_p}\left(\frac{\partial V}{\partial x}+\frac{\partial U}{\partial y}\right)$$

where:
h_p is vertical coordinate of the location of the free flow surface. (It is also equal to the depth of the stream when the zero of the vertical axis is located at the bottom of the stream), meter,
$z=o$ is vertical coordinate of the location of the bottom of the stream equal to zero, meter,
V is first horizontal component of the flow velocity vector, averaged on the vertical, $\frac{meter}{sec}$,
U is second horizontal component of the flow velocity vector, averaged on the vertical, $\frac{meter}{sec}$,
ρ is density of water, $\frac{kg}{meter^3}$,
K_z is coefficient of proportionality, $\frac{meter}{sec}$,
D_v is kinematic viscosity of water, $\frac{meter^2}{sec}$.
In the terms $K_z\cdot\frac{V}{h^2}$, $K_z\cdot\frac{U}{h^2}$ the second power at the average flow depth appeared due to double vertical integration from the bottom to the free surface and applying the theorem on the mean value of a certain integral.
Undoubtedly, solving a system of equations is a very complex hydromechanical problem. But the specificity of the tasks set is such that the solution of system (3) can be significantly simplified. First of all, we are not particularly interested in the distribution of water velocities in the river. For our purposes, it is sufficient to know the average velocity of water in the river and the area of the living section of the water flow in the river.
Thus, our task is reduced to solving only the first equation from the system (3), provided that the velocity distribution diagram across the movement of water in the river is known. That is, the pollution spot's distribution over the river's surface will be determined by solving equation (4).

$$\frac{\partial S}{\partial t}+\frac{\partial(S\cdot V)}{\partial x}+\frac{\partial(S\cdot U)}{\partial y}=+\frac{\partial D_s \partial S}{(\partial x)^2}+\frac{\partial D_s \partial S}{(\partial y)^2}+\mathrm{I} \quad (4)$$

If we calculate the transformation of the pollution spot under the steady flow of the river (average flow rates do not change for a long time), then

$$\frac{\partial V}{\partial x}+\frac{\partial U}{\partial y}=0 \quad (5)$$

Since the position of the water surface does not change

$$\frac{\partial h_p}{\partial t}=0. \quad (6)$$

In addition, the existence of a transverse component of the average flow velocities can be neglected. The pulsating turbulent part of the transverse velocities will be considered through the water flow dispersion.
Equation (4) can be slightly simplified

$$\frac{\partial S}{\partial t}+V\cdot\frac{\partial S}{\partial x}=\frac{\partial D_s \partial S}{(\partial x)^2}+\frac{\partial D_s \partial S}{(\partial y)^2}+\mathrm{I} \quad (7)$$

But even in this case, solving the equation is difficult.

To solve it, it will be necessary to find conservative and transport approximations of finite differences for all differential terms of the equation. After that, you will have to find a stable solution using an explicit or implicit scheme, provided the calculation is done with a time step closest to the Courant-Levy condition [31]. The maximum approximation to the upper limit of the Courant Levy condition makes it possible to reduce the manifestation of "parasitic" schematic viscosity in calculations. Let us determine the value D_s responsible for the spread of the pollution spot by diffusion. According to the research of Velikanov M.A.[32]

There is a relationship between the velocity dispersion and the velocity of a continuous medium (water) according to the Karaushev formula (8) [32].

$$D_s = \frac{g \cdot h_p \cdot V}{(0.7 \cdot C + 6) \cdot C} \tag{8}$$

where,
h_p is depth of water flow, meter,
g is free-fall acceleration equal to $9.81 \frac{meter}{sec^2}$,
C is Shezy coefficient, approximately equal to 50 $\frac{meter^{1/2}}{sec}$ for lowland rivers flowing in a fairly flat wide channel. Here and below, the Shezy coefficient is assumed to be $50 \frac{meter^{1/2}}{sec}$.

Let us set the velocity field in the river by a parabola. On the banks of the river, we set the speed equal to zero. We calculate the average speed of water movement and the depth of the flow through the flow of water, the slope of the bottom, and the width of the river, which is quite stable.

If we assume a parabolic diagram of velocities on the cross-section of the river, then the average value of the speed will be two-thirds of the maximum speed (9)

$$V_{av} = \left(\frac{2}{3} \cdot V_{max}\right) \tag{9}$$

And the regularity of velocity distribution across the flow is approximated by the formula

$$\mathrm{V(y)} = \frac{-4 \cdot (V_{max}) \cdot y^2}{B^2} + (V_{max}) \tag{10}$$

Regularity (9) and (10) allow us to determine the coefficient of turbulent diffusion on the cross-section of the river according to the formula (8)

$$D_s = \frac{g \cdot h_p \cdot \left(\frac{-4 \cdot (V_{max}) \cdot y^2}{B^2} + \left(\frac{3}{2} \cdot V_{av}\right)\right)}{(0.7 \cdot C + 6) \cdot C} = \frac{g \cdot h_p \cdot \left(\frac{-4 \cdot \left(\frac{3}{2} \cdot V_{av}\right) \cdot y^2}{B^2} + \left(\frac{3}{2} \cdot V_{av}\right)\right)}{(0.7 \cdot C + 6) \cdot C} \tag{11}$$

We will identically transform formula (11) to a form that will be convenient for calculation and will rely only on the usual initial parameters (water discharge - Q, channel width - B, bottom slope - I). We write the Chezy equation (12)

$$V_{av} = C \cdot \sqrt{h_p I} \tag{12}$$

where,

I is slope of the river bottom, defined as the ratio of the fall of the bottom marks in the river section and the length of the river section (dimensionless value),

C is Shezy coefficient, taken equal to 50 $50 \frac{meter^{1/2}}{sec}$.

Let us substitute the speed determined through the flow depth into expression (11).

$$D_s = \frac{g \cdot h_p \cdot \left(\frac{-4 \cdot \left(\frac{3}{2} \cdot C \cdot \sqrt{h_p\, I}\right) \cdot y^2}{B^2} + \left(\frac{3}{2} \cdot C \cdot \sqrt{h_p\, I}\right) \right)}{(0.7 \cdot C + 6) \cdot C} \quad (13)$$

Let us now determine the relationship between the flow depth and water discharge for a fixed flow width, a given bottom slope, and some assumptions about the shape of the channel cross section in the areas of impurity discharge.

$$Q = \omega \cdot C \cdot \sqrt{R\, I} \quad (14)$$

For wide shallow riverbeds

$$h_p \approx R \quad (15)$$

The open area of a wide and shallow channel with the accepted approximation (15) is calculated by the formula (17) since, by definition, the hydraulic radius is equal to the quotient of the area of the open section divided by the wetted perimeter (16).

$$R = \frac{\omega}{(B + 2 \cdot \mathrm{h_p})} \quad (16)$$

and under the condition $h_p \approx R$ (see.15) and the condition $\mathrm{h_p}$ "B we get

$$\omega \approx \mathrm{B} \cdot \mathrm{h_p} \quad (17)$$

and correspondingly

$$Q = B \cdot h_p \cdot C \cdot \sqrt{h_p\, I} \quad (18)$$

Where should

$$h_p = \left(\frac{Q}{B \cdot C \cdot \sqrt{i}}\right)^{\frac{2}{3}} \quad (19)$$

The formula for determining the turbulent diffusion coefficient is determined by expression (20). Equations (13) and (19) are used.

$$D_s = \frac{g \cdot \left(\frac{Q}{B \cdot C \cdot \sqrt{i}}\right)^{\frac{2}{3}} \cdot \left(\frac{-4 \cdot \left(\frac{3}{2} \cdot C \cdot \sqrt{\left(\frac{Q}{B \cdot C \cdot \sqrt{i}}\right)^{\frac{2}{3}} \cdot I}\right) \cdot y^2}{B^2} + \left(\frac{3}{2} \cdot C \cdot \sqrt{\left(\frac{Q}{B \cdot C \cdot \sqrt{i}}\right)^{\frac{2}{3}} \cdot I}\right) \right)}{(0.7 \cdot C + 6) \cdot C} \quad (20)$$

As an example, Figure (1) shows the distribution of the diffusion coefficient across the river in the discharge zone with a river width of 10 meters, a flow rate of 20 $\frac{meter^3}{sec}$ and a river slope of 0.001.

The flow depth is calculated by the formula (19): $h_p = 1.1696$ m.

Average speed according to the formula (12): $V = 1.71 \ \frac{meter}{sec}$.
The approximation of flow velocities across the channel will be reflected by formula (10).

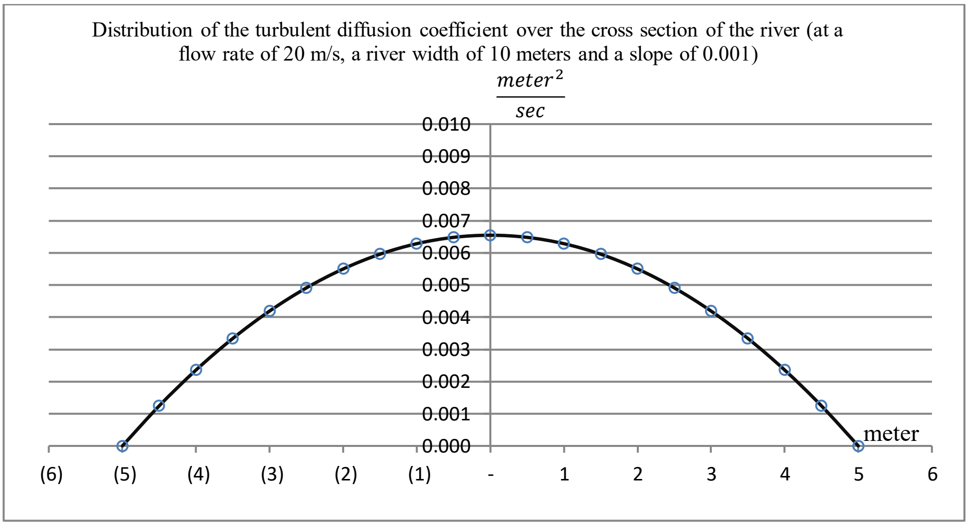

Fig.1. Diagram of distribution of turbulent diffusion coefficient on cross-section of river with slope of 0.001, river width of 10 meters, and discharge of $20\frac{meter^3}{meter}$.

The results obtained are very close to the results of other authors obtained for lowland rivers [35]. Similarly, distribution diagrams of turbulent diffusion coefficients were calculated for all design objects. For all rivers in the spillway construction zone, the Shezy coefficient was taken to equal 50. The width of the rivers in the spillway area was determined from maps and indicated at the beginning of the calculation of each object.
Computational Finite-Difference Schemes. The main equation responsible for the spread of the pollution spot is equation (7). This is an evolutionary (non-stationary) equation of the second order, spatially two-dimensional.
Let us write equation (7) again for ease of reading the material.

$$\frac{\partial S}{\partial t} + V \cdot \frac{\partial S}{\partial x} = \frac{\partial D_s \partial S}{(\partial x)^2} + \frac{\partial D_s \partial S}{(\partial y)^2} + \mathrm{I}$$

It is supposed to be solved using explicit finite difference schemes. Recall that explicit schemes are schemes in which the unknown value of the desired variable, independent of its environment at the calculated time, is based on the past state of the variable itself and its environment.

For the evolutionary part (time derivative), the finite difference scheme will be used

$$\frac{\partial S}{\partial t} \backsim \frac{S_{i,j}^{t+1} - S_{i,j}^{t}}{\Delta t} \qquad (21)$$

For the convection term, the finite difference scheme will be used

$$V \cdot \frac{\partial S}{\partial x} \backsim V_{i,j}^{t} \frac{S_{i,j}^{t} - S_{i-1,j}^{t}}{\Delta x} \qquad (22)$$

The fact that water movement in the river occurs in the same direction is used. The coordinate axis is chosen so that the speed will always be positive. Of course, in objects in which water moves in different directions as a result of whirlpools, the approximation will be more difficult. This approximation, well studied, has an official name - "directed differences scheme"- and is stable and conservative (incapable of causing the appearance of non-existent quantities of the transported substance). The main restriction on this scheme is the Courant-Levy restriction on the ratio of steps in time and space when choosing them.

$$\frac{\Delta x}{\Delta t} \geqslant V_{i,j}^{t} \tag{23}$$

The terms responsible for the transfer of matter due to turbulent diffusion are of particular interest.

$$\frac{\partial D_s \partial S}{\partial x^2} + \frac{\partial D_s \partial S}{\partial y^2} \tag{24}$$

$$\frac{\partial D_s \partial S}{\partial x^2} + \frac{\partial D_s \partial S}{\partial y^2} = D_s \cdot \frac{\partial^2 S}{\partial x^2} + D_s \cdot \frac{\partial^2 S}{\partial y^2} + \frac{\partial D_s}{\partial x} \cdot \frac{\partial S}{\partial x} + \frac{\partial D_s}{\partial y} \cdot \frac{\partial S}{\partial y} \tag{25}$$

For the first and second terms on the right side of equality (25), there is a single, generally accepted, conservative, stable calculation scheme.

$$D_s \cdot \frac{\partial^2 S}{\partial x^2} + D_s \cdot \frac{\partial^2 S}{\partial y^2} \backsim D_{s}{}_{i,j}^{t} \cdot \frac{S_{i+1,j}^{t} - 2S_{i,j}^{t} + S_{i-1,j}^{t}}{\Delta x^2} + D_{s}{}_{i,j}^{t} \cdot \frac{S_{i,j+1}^{t} - 2S_{i,j}^{t} + S_{i,j-1}^{t}}{\Delta y^2} \tag{26}$$

Certainly, the Courant-Levy condition also applies here, but in a slightly different form

$$\Delta\, t \leqslant \frac{\Delta y^2}{D_s} \tag{27}$$

Regarding the third and fourth terms on the right side of equality (25), we can say that it is possible to make a non-conservative form of approximation, but it is completely unstable in calculations. Taken in isolation, these terms give rise to "jagged" static instabilities, ultimately leading to the crash of calculations. The result of the solution can only be achieved because the second and third terms on the right side of equality (25) smooth and suppress the oscillating effect from the third and fourth terms on the right side of equality (25). Note that the third term on the right side of equality (25) equals zero; the current is steady since the channel is straight. This means there is no dispersion gradient at a given distance from the coast and along the river. That is

$$\frac{\partial D_s}{\partial x} = 0$$

The following approximation of the fourth term in equality (25) was used in the calculations.

$$\frac{\partial D_s}{\partial y} \cdot \frac{\partial S}{\partial y} \backsim \frac{D_{s}{}_{i,j}^{t} + D_{s}{}_{i,j-1}^{t}}{\Delta y} \cdot \frac{S_{i,j}^{t} + S_{i-1,j}^{t}}{\Delta y} - \frac{D_{s}{}_{i,j+1}^{t} + D_{s}{}_{i,j}^{t}}{\Delta y} \cdot \frac{S_{i,j+1}^{t} + S_{i,j}^{t}}{\Delta y}$$

The source term - "I" in equation (7) does not raise questions in the calculation.

4 Conclusions

1. The most informative formulas for calculating turbulence characteristics in riverbeds and channels are selected based on analyzing and comparing the most common formulas for calculating turbulence coefficients in a water flow.
2. Finite-difference analogs of equations for calculating the impurity propagation in a water stream are constructed. The proposed schemes allow us to design computational algorithms using classical approaches for solving impurity transfer equations with variable turbulent exchange coefficients.
3. A mathematical model has been developed that allows calculating the spread of impurities in a water stream, considering the variability of the turbulent exchange coefficients.

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