Mathematical modelling of hydrochemical processes in surface waters

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Abstract. In recent years, a large number of mathematical models of water quality have been developed which can be used for predictive calculations under certain conditions. This work is mainly devoted to the mechanical aspects of substances transport in watercourse systems. It is practically possible to quickly determine the concentration of impurities in a river only by methods of mathematical modelling of impurities transport.

Introduction

Intensive economic use of water sources and increased quality requirements for the water taken from the resources pose a number of tasks due to the correct solution which determines the environmental safety of water bodies.

The most important of these are:

• Assessment of pollutants concentrations in water bodies
• Study of the pollutants spread due to the anthropogenic factors and special engineering measures necessary to regulate water quality, both in water bodies and at water intakes
• Assessment of the actual state of water quality of the water source and forecast of its change.

On the one hand, sufficient accuracy in solving these problems is necessary for design and operational practice, and the high efficiency which makes it possible to carry out mass calculations of the objects under study and evaluate the possible development of the situation.

In recent years, a large number of methods for mathematical modelling of water quality have been developed, which can be used for predictive calculations under certain conditions.

Currently, the most effective way to combine these properties can be done by express methods, i.e. methods that allow you to quickly and with sufficient accuracy for practical purposes to determine the speed of distribution and concentration of pollutants in water bodies and watercourses, i.e. make a forecast of the development of the situation and propose measures to prevent the spread of pollution, its localization and, ultimately, the prevention of damage to both the natural environment and the economy.

Engineering problems in environmental practice often require fast, well-informed decision making. However, the available modern tools do not make it possible. Widespread

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mathematical modelling, even with the use of personal computers, requires a significant amount of time to prepare the initial data in any case. On the other hand, practice most often does not require the use of accurate modelling, the exact match of the models used to the actually occurring processes. As noted in [2], there are a large number of models of varying complexity that can be used to study the spread of pollutants in water bodies, the limits of applicability of models have been investigated, and recommendations have been developed for their practical application.

With the development of human society and the depletion of water resources, attitudes towards water have been changed. Until the beginning of the 20th century, the water of rivers, lakes and underground sources were considered as a “free gift of nature”, and the rivers themselves were also considered as a convenient form of waste disposal. At present, clean fresh water, limiting the development of irrigated agriculture and water-intensive industries, municipal domestic water supply is assessed as one of the most important natural resources stimulating the development of the economy and culture, and improving the welfare of the people.

Operational determination of impurities in the river is possible practically only by the method of mathematical modelling of impurities transfer. Changes of impurity concentration are not only due to the dilution, but also due to the effects of sorption, absorption, photosynthesis, etc. These processes are very common, sometimes prevailing, especially at low flow rates [1-5].

In this work, the members of concentrated and distributed inflows and outflows of water and salt were derived into the corresponding equations earlier by Yu. M. Denisov and M. Ziyakhodzhaev in 1976 and used by Denisov and Sergeev in 1992.

Impurities enter the river from concentrated and distributed sources. Then they are carried by the flow, diluted, participate in various transformations, interact with each other and the flow boundaries.

In this paper, the impurities transport in watercourse systems is considered in a one-dimensional formulation. The inhomogeneous equation of hydrodynamics and turbulent diffusion is used as the initial equations for the transfer of non-conservative impurities.

The $s$ the length of the river from the chosen reference point is denoted, $u(s,t)$ the average velocity along the area of water section of the flow $\omega(s,t)$ over distances $s$ at a time $t$ [7-15].

![Fig.1](image)

**Fig.1** Scheme for the derivation of the water balance equation and the mass balance of the k-th substance in the river, taking into account concentrated and distributed inflows and outflows.
The flow of $k$ th substance through a unit area of water section $q_{ck}(s,t)$ is equal to

$$q_{ck}(s,t) = C_k u - K_T \frac{\partial C_k}{\partial s}$$

(1)

Where, $C_k u$ – convective flow of the component; $K_T \frac{\partial C_k}{\partial s}$ - diffusion part of the flow.

During the time $dt$, as a result of the movement of $k$ th substance in the volume of $\omega ds$, its equal amount will be accumulated. Then

$$\left[ \alpha q_{ck} - (\alpha q_{ck} + \frac{\partial \alpha q_{ck}}{\partial s}) \right]ds \cdot dt = - \frac{\partial q_{ck}}{\partial s} \cdot \omega ds dt$$

In the area of consideration, $k$ th substance can enter along with precipitation

$$C_{ks} \cdot a_x B ds dt$$

Where, $C_{ks}$ - concentration of $k$ th substance in sediments; $a_x$ - their intensity; $B$ is the width of the flow along the edges.

In addition, the substance under consideration can enter the river section with a surface lateral distributed flow:

$$C_{knp} q ds dt$$

Here, $C_{knp}$ the concentration of $k$ is that substance in the surface distributed lateral inflow. The inflow or outflow of a substance occurs in the form of salt exchange between the river and groundwater with intensity $i_{\phi}$.

This value is

$$C_{k_{phi}}^{*} i_{\phi} \chi ds dt,$$

Where:

$$C_{k_{phi}}^{*} = \begin{cases} C_k for & i_{\phi} \geq 0 \\ C_{kg} for & i_{\phi} \leq 0 \end{cases}$$

$C_{kg}$ – concentration of $k$ th substance in groundwater.

The intensity of filtration if is considered positive when water is filtered from the river into the ground.

The substance under consideration can enter or leave the river through concentrated inflows and outflows.

$$\sum_i C_{kni} Q_{ni}(s,t) \delta(s-s_{ni})ds dt - \sum C_{komj} Q_{omj}(s,t) \delta(s-s_{omj})ds dt$$

Here $C_{kni}$ and $C_{komj}$ are the concentration of pollutants in inflows and outflows. Finally, as a result of chemical reactions, a substance can turn into $p$. 
\[ - \sum_p \eta_{kp}(s,t) \omega ds dt \]

Here - \( \eta_{kp} \) the intensity of the transition to \( k \) that substance in \( p \) in a unit of volume per unit of time. Besides it \( \eta_{kp} = -\eta_{pk} \)

All the above leads to their change in the mass of the \( k \) substance in volume over time:

\[ \frac{\partial C_k \omega}{\partial t} \]

Collecting all the balance members and equating them to the last expression we obtain the following equation for the balance of \( k \) th substance in differential form

\[
\frac{\partial C_k \omega}{\partial t} + \frac{\partial}{\partial s} \left( C_k u - K_T \frac{\partial C_k}{\partial s} \right) = \sum_i C_{kiu} Q_{iu} \delta(s - s_i) - \sum_j C_{kj} Q_{j} \delta(s - s_j) + C_k \alpha_s B + C_{kp} q_{up} - C_{kp} \dot{q}_p - \sum_b \eta_{bk}(s,t) \omega
\]

(2)

Here, \( K_T \) is the turbulence coefficient.

Equation (2) can be simplified as it has been done in [ ] by using the water balance equation (3).

\[
\frac{\partial \omega}{\partial t} + \frac{\partial \omega u}{\partial s} = (\alpha_s - E) B(s,t) - i_s \dot{X} + q_{pwm} + \left[ \sum_{i=1}^n Q_{iu}(s,t) \delta(s - s_{mi}) - \sum_{j=1}^n Q_{j} \delta(s - s_{mj}) \right]
\]

(3)

For this, we write it in the following expression:

\[
\alpha_s \left( \frac{\partial C_k}{\partial t} + u \frac{\partial C_k}{\partial s} \right) + C_k \left( \frac{\partial \omega}{\partial t} + \frac{\partial \omega u}{\partial s} \right) = \frac{\partial}{\partial s} \left( K_T \omega \frac{\partial C_k}{\partial s} \right) + \sum_i C_{kiu} Q_{iu} \delta(s - s_i) - \sum_j C_{kj} Q_{j} \delta(s - s_j) + C_k \alpha_s B + C_{kp} q_{pm} - C_{kp} \dot{q}_p \dot{X} + \sum_b \eta_{bk} \omega
\]

(4)

Given the expression (3) and the second bracket on the left side (4) we get the following:

\[
\alpha_s \left( \frac{\partial C_k}{\partial t} + u \frac{\partial C_k}{\partial s} \right) = \frac{\partial}{\partial s} \left( K_T \omega \frac{\partial C_k}{\partial s} \right) + \sum_i (C_{ki} - C_k) Q_{iu} \delta(s - s_i) - B \left[ (C_k - C_k) \alpha_s - C_k E \right] + (C_{kp} - C_k) q_{pm} + (C - C_k) \dot{q}_p \dot{X} + \sum_b \eta_{bk} \omega
\]

(5)

Or
\[
\frac{\partial C_k}{\partial t} = \frac{1}{\omega} \frac{\partial}{\partial s} \left( K_r \omega \frac{\partial C_k}{\partial s} \right) - u \frac{\partial C_k}{\partial s} - \frac{1}{\omega} \left[ \sum_i Q_m \delta(s - s_i) + B(a_x - E) + q_{pm} - i_x \varphi \right] C_k + \\
+ \frac{1}{\omega} \left[ \sum C_{ks} Q_m \delta(s - s_i) + BC_{ks}a_x + C_{pm}q_{pm} \right] - \frac{1}{\omega} C_{ks}^\varphi i_x \varphi X + \sum \eta_{nk}
\] 

Equation (6) is a partial differential equation of parabolic type with respect to the desired concentration of the \( k \) th substance in the river.

This concentration is found by numerically solving equation (6) by the sweep method and adapting it to the specific conditions of the medium under considering case.

**Conclusion**

The influence of physical characteristics such as temperature and salinity on changes in water quality is very important. As far as chemical processes are concerned, they play a big role in water pollution. Our study proved that water quality can be modeled and studied using mathematical modeling, and many parameters can be obtained in a relatively limited time. Such studies without the use of mathematical modelling can be very time consuming and may require many researchers to spend a lot of time in the field. Thanks to mathematical models, results and conclusions can be drawn easily and in a short time.

This model takes into account the transport of minerals and chemicals, the influence of the ionic composition of water on density and diffusion, the transport, absorption and release of nutrients by phytoplankton, as well as the cycles of phosphorus, nitrogen and silicon and other pollutants. Thanks to the analytical study through the model, it is possible to obtain inequalities that ensure the existence and uniqueness of the solution to the problem.

Theoretical estimates of acceleration and efficiency of parallel algorithms are obtained. This is intended for mathematical calculations of possible scenarios for the development of waters with complex impurities.

**References**


