MATHEMATICAL DESCRIPTION OF THE PHYSICAL PROCESS OF FORMING THE SURFACE WATERS QUALITY

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ABSTRACT

Research goal of the paper is mathematical description of the physical process of forming the surface waters quality on the example of the Lower Section of the Ingulets River.

The methodology in which the chemical status of a water body (category and class of water quality) is assessed based on the analysis of observational data (concentrations of priority hazardous pollutants) was used. Based on a general assessment, the suitability of surface waters for use in various economic purposes is established.

We propose to represent dependence of the category of water quality on the concentration of hydrochemical ingredients in the form of regression equations. The article provides examples of such a representation of the dependencies of the water quality categories on the values of hydrochemical ingredients for the Lower Section of the Ingulets River.

An environmental assessment of the surface waters quality of the Lower Section of the Ingulets River was carried out on the basis of the analysis of hydrochemical ingredients in accordance with the fishery standards for the observation period of 2018 year with subsequent calculation and generalization. The results can serve as a basis for visualizing the results of modeling the ecological state of surface waters using GIS technologies, determining the impact of anthropogenic load on ecosystems of water bodies, estimating changes of water quality, informing the public, solving economic and social issues, related to the rational use of natural resources and ensuring environmental protection.

Keywords: mathematical model, physical process, water quality, surface waters, hydrochemical ingredients

INTRODUCTION

The quality of surface waters is a certain external characteristic of a water body, which makes it possible to assess the possibility of its use for one or another practical purpose, which can be represented by a scale of some continuous or discrete indicator. Physical, hydrochemical and hydrobiological processes that affect the formation of water quality

in a river depend on the intensity of mixing of water. Dynamic (turbulent) mixing arising in the presence of vertical and horizontal velocity gradients is the most powerful factor affecting water masses [1]. Intensive water exchange provides active circulation of water, activates the processes of self-purification of surface waters and improves their quality. The problem of preserving the quality of natural waters is complicated by the fact that the volume of industrial and domestic wastewater, which is often discharged into rivers without sufficient treatment, is increasing sharply.

Churuksaeva V.V. and Starchenko A.V. [2] offer for calculating the spread of pollutants the mathematical model that includes the continuity equation:

$$\frac{\partial(h\bar{u})}{\partial x}+\frac{\partial(h\bar{v})}{\partial y}=0, \tag{1}$$

equations of motion:

$$\frac{\partial(h\bar{u}^2)}{\partial x}+\frac{\partial(h\bar{u}\bar{v})}{\partial y}=-gh\frac{\partial(z_b+h)}{\partial x}+\frac{1}{\rho}\frac{\partial(h\bar{\tau}_{xx})}{\partial x}+\frac{1}{\rho}\frac{\partial(h\bar{\tau}_{xy})}{\partial y}+\frac{(\tau_{xz})_s-(\tau_{xz})_b}{\rho}-h\bar{F}_x, \tag{2}$$

$$\frac{\partial(h\bar{u}\bar{v})}{\partial x}+\frac{\partial(h\bar{v}^2)}{\partial y}=-gh\frac{\partial(z_b+h)}{\partial y}+\frac{1}{\rho}\frac{\partial(h\bar{\tau}_{yx})}{\partial x}+\frac{1}{\rho}\frac{\partial(h\bar{\tau}_{yy})}{\partial y}+\frac{(\tau_{yz})_s-(\tau_{yz})_b}{\rho}-h\bar{F}_y \tag{3}$$

and the equation for the transfer of concentration of pollutant:

$$\frac{\partial(h\bar{u}\bar{c})}{\partial x}+\frac{\partial(h\bar{v}\bar{c})}{\partial y}=\frac{\partial(h\bar{q}_x)}{\partial x}+\frac{\partial(h\bar{q}_y)}{\partial y}+((q_z)_s-(q_z)_b)+S, \tag{4}$$

where $h(x,y)$ – depth; $\bar{u}(x,y),\bar{v}(x,y)$ – values of the components of the velocity vector $\vec{w}=(u,v)$ averaged over depth; $z_b(x,y)$ – topography bottom; ρ – density of water, $g=9.81$ m/s^2 – acceleration of gravity; $\bar{\tau}_{xx},\bar{\tau}_{xy},\bar{\tau}_{yx},\bar{\tau}_{yy}$ – components of the tensor of viscous stresses and Reynolds stresses averaged over depth; $(\tau_{xz})_s,(\tau_{xz})_b,(\tau_{yz})_s,(\tau_{yz})_b$ – friction on the surface of the river and its bottom, respectively; $\bar{F}_x,\bar{F}_y$ – components of the Coriolis force averaged over depth; $\bar{c}$ – concentration of pollutant averaged over depth; $\bar{q}_x,\bar{q}_y$ – diffuse and turbulent flows of mass; S – source of pollution; $(q_z)_s,(q_z)_b$ – flows of pollution on the surface and bottom, respectively.

In the mathematical model proposed by the authors [2], speed of pollutants coincides with the velocity of river stream and their concentration in water is relatively low. In addition, the authors simulate the distribution of pollutants of a relatively small mass (compared with the mass of flowing water) entering the river at a low velocity. And it is assumed that near the release there are no three-dimensional turbulent effects.

The semi-empirical equation of turbulent diffusion of any pollutant for three-dimensional space is represented by R.V. Ozmidov as follows [3]:

$$\frac{\partial\bar{C}_i}{\partial t}+\bar{u}\frac{\partial\bar{C}_i}{\partial x}+\bar{v}\frac{\partial\bar{C}_i}{\partial y}+\bar{w}\frac{\partial\bar{C}_i}{\partial z}=K_L\left(\frac{\partial^2\bar{C}_i}{\partial x^2}+\frac{\partial^2\bar{C}_i}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(K_Z\frac{\partial\bar{C}_i}{\partial z}\right), \tag{5}$$

where K_L и K_Z – coefficients of horizontal and vertical turbulent diffusion; $\overline{u},\overline{v},\overline{w}$ – averaged over coordinates x, y, z velocity components; $\overline{C_i}$ – concentration of pollutant.

In practice, when solving diffuse problems, modernized versions of the equation are often used that take into account the initial and boundary conditions, water body morphometry, hydraulic flow conditions and the specifics of the process energy supply [1, 4-6].

The method of environmental assessment of surface water quality according to the relevant categories [7] allows analyzing observational data, determining the classes and categories of water quality, the state of water bodies, and assessing the conditions for the restoration of water resources using many tables. Environmental assessment can be performed on an extended and reduced list of indicators. The reduced list involves the use of a compulsory minimum of information on indicators that are constantly determined on the state water monitoring network of Ukraine.

The initial data for assessing the ecological state of waters in the Lower Section of the Ingulets River are the results of analytical control of surface waters by the State Ecological Inspectorate in Kherson region: 1 – the Ingulets River – village Arkhanhel's'ke (210 km from the mouth), 2 – the Ingulets River – village Kalynivs'ke (124 km from the mouth), 3 – the Ingulets River – village Dar'ivka (20 km from the mouth) and the State Ecological Inspectorate in Mykolaiv region: 4 – the Ingulets River – town Snigurivka (100 km from the mouth).

The results of recent studies of the surface waters of the Lower Section of the Ingulets River indicate constant water pollution and excess maximum permissible concentrations (MPC) of substances (COD, Suspended solids, Chlorides, Sulphates, BOD_5, Phosphates, Nitrites and SAS) (fig. 1).

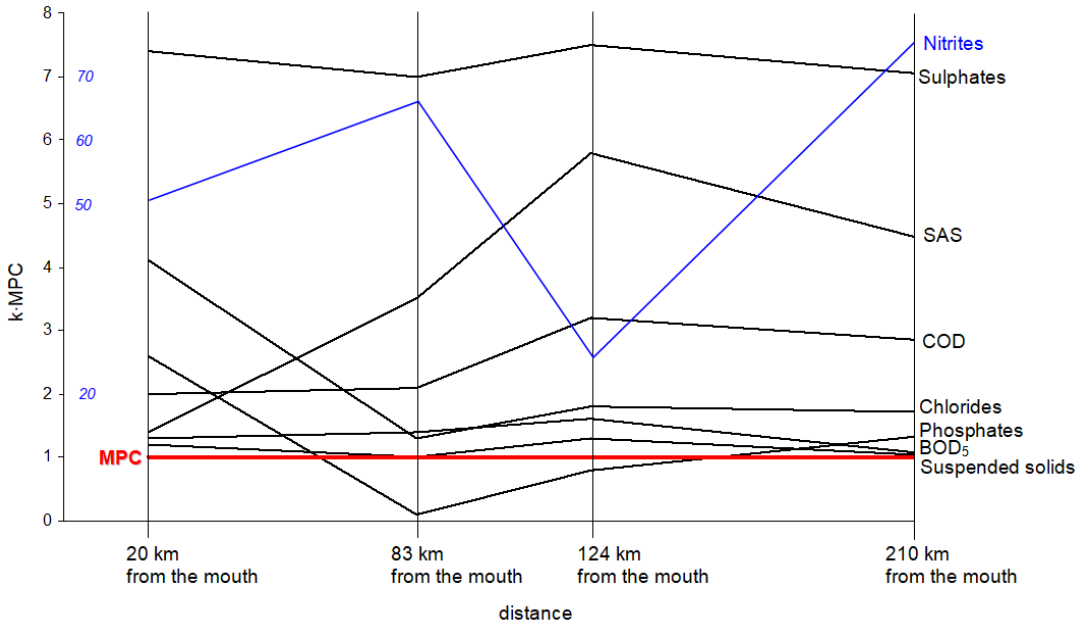

Figure 1 – Excess annual average values (2018) of hydrochemical ingredients relative to MPC of the Lower Section of the Ingulets River

Elementary signs of water quality are hydrochemical ingredients, by which surface waters quality assessment can be performed. We propose to express the dependence of the category of water quality on the concentration of hydrochemical ingredients in the form of a regression equation. The following are examples of such a representation of the dependencies of the water quality categories on the values of Chemical oxygen demand (COD), Suspended solids, Chlorides, Sulphates, Synthetic surfactants (SAS) (fig. 2), Biological oxygen demand (BOD_5), Phosphates and Nitrites (fig. 3).

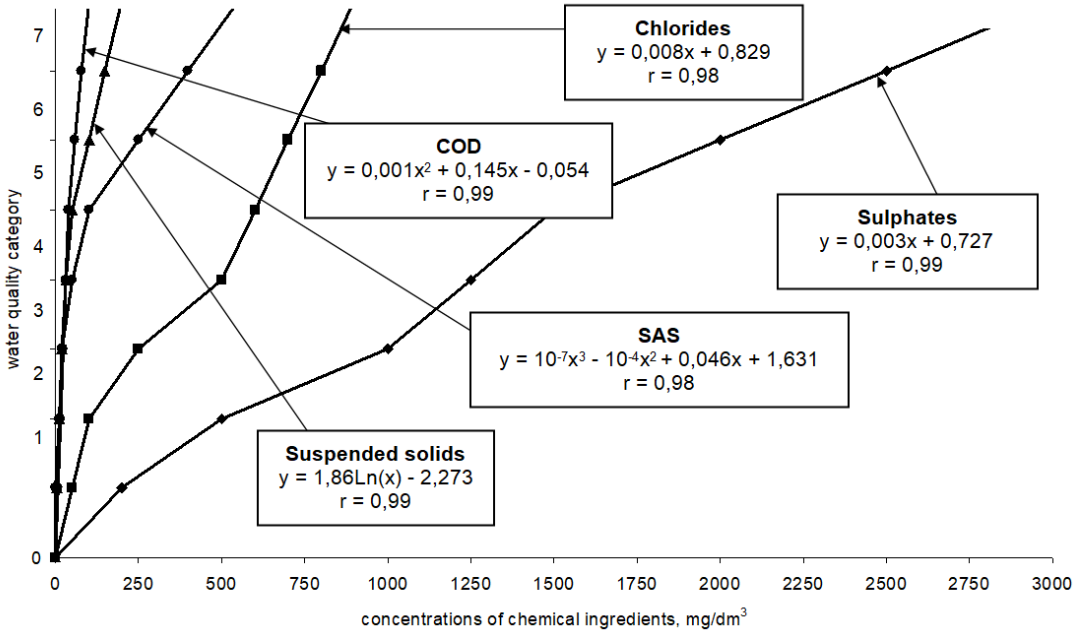

Figure 2 – Dependence of the category of surface water quality on the concentration of hydrochemical ingredients (COD, Suspended solids, Chlorides, Sulphates, SAS)

As a result of constructing approximating curves according to the values of the concentrations of hydrochemical ingredients, regression equations are obtained. They are logarithmic and polynomial dependencies (fig. 2, 3). The dependency equations are characterized by the values of the correlation coefficients from 0.98 to 0.99, which indicates the presence of close connections between the values of the provided sample. The obtained dependences provide an opportunity to determine the category of surface water quality (vertical axis) based on measured concentrations of the corresponding hydrochemical ingredients (horizontal axis). They can serve as a basis for assessment of the quality of the surface waters of the Lower Section of the Ingulets River and visualizing the results of modeling the ecological state of surface waters.

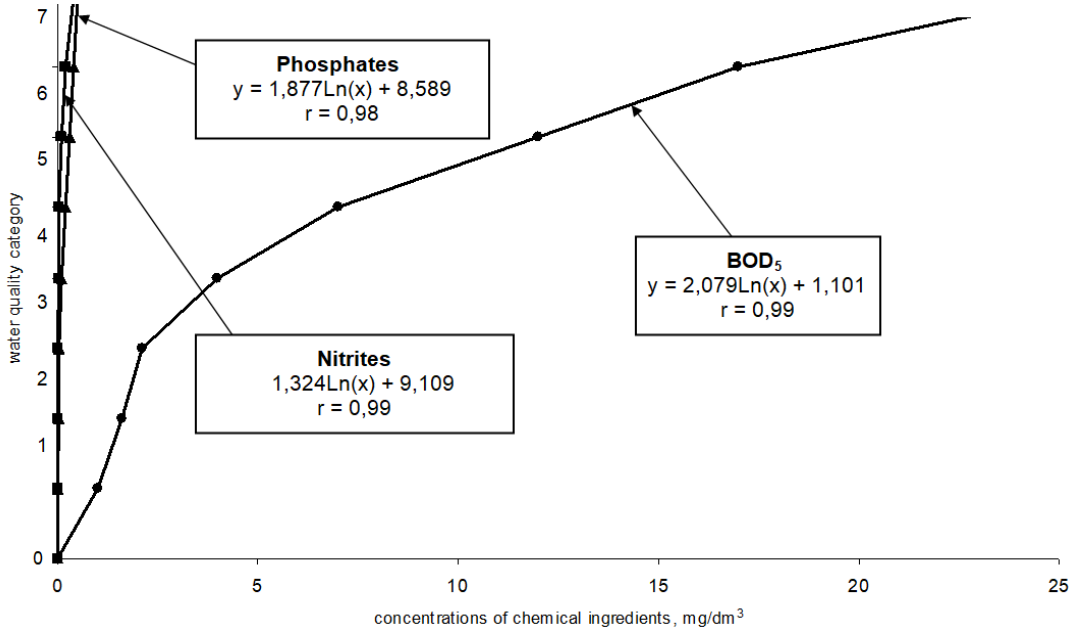

Figure 3 – Dependence of the category of surface water quality on the concentration of hydrochemical ingredients (BOD_5, Phosphates and Nitrites)

An assessment of the quality of the surface waters of the Lower Section of the Ingulets River (village Dar'ivka) was carried out on the basis of the analysis of hydrochemical ingredients for the observation period for 2018 following to the fishery norms and presented in table 1.

Table 1 – Water quality assessment of the Ingulets River – village Dar'ivka (20 km from the mouth) by the ecological classification for 2018 following to the fishery norms

Parameter	C_i, mg/dm^3	MPC, mg/dm^3	Water quality category	Water quality class	Water condition	The extent of water purity
Suspended solids	24.0	20.0	4	III	acceptable	poorly contaminated
BOD_5	4.0	3.0	4	III	acceptable	poorly contaminated
Nitrites	4.00	0.08	7	V	very poor	very contaminated
SAS	1.40	0.50	2	II	very good	clean
Chlorides	1229	300	7	V	very poor	very contaminated
Sulphates	736	100	3	II	good	sufficient clean
COD	27.2	20.0	4	III	acceptable	poorly contaminated
Phosphates	9.0	3.5	7	V	very poor	very contaminated

The table data demonstrate the ecological state of the surface waters of the Lower Section of the Ingulets River, which varies from "very good" by SAS (Class II, Category 2, clean) to "very poor" by Nitrites, Chlorides, Phosphates (Class V, Category 7, very contaminated water) (tabl. 1). The unstable ecological state [8] and the change in the water quality of the Lower Section of the Ingulets River are explained by the flow of polluted water into the Ingulets River.

For the Lower Section of the Ingulets River, excess of the maximum permissible concentration for Nitrites, Chlorides, Phosphates and other substances are most often observed, which indicates that the main source of pollution is discharges of highly mineralized polluted industrial effluents of the city Kryvyi Rih serving the mining, metallurgical and chemical industries. 8 of 11 Ukrainian enterprises for the extraction and processing of iron ore are located in the Kryvyi Rih basin. Here are enterprises serving the metallurgical industry – one of the world's largest metallurgical plants (PJSC "ArcelorMitall Kryvyi Rih"), five mining and processing combines (MPC) – Pivnichnyi MPC (PivnMPC), Pivdennyi MPC (PivdMPC), Cental'nyi MPC (CMPC), Novokryvoriz'ky MPC (NKMPC), Ingulets'kiy MPC (InMPC), three ore repair plants.

The volume of wastewater of enterprises reaches millions of cubic meters per year, which negatively affects the quality of the water of the Ingulets River, which carries its polluted water to the Lower Section of the Dnieper River.

An analysis of the results of the study suggests that it is necessary to use more efficient wastewater treatment plants at Kryvbas enterprises. The introduction of modern technologies for the production of products with a closed water cycle will reduce the amount of pollutants in the source of their formation.

CONCLUSION

The mathematical description (presentation) of assessing the surface waters quality of the Lower Section of the Ingulets River in accordance with the fishery standards based on the methodology for assessing water quality by hydrochemical parameters was performed. Ecological state of the surface waters of the Lower Section of the Ingulets River varies from "very good" by SAS (Class II, Category 2, clean) to "very poor" by Nitrites, Chlorides, Phosphates (Class V, Category 7, very contaminated water).

The qualification of the ecological state of the Lower Section of the Ingulets River determines the necessity to carry out environmental protection activities in the ecosystem (for example, installation of effective wastewater treatment plants, the introduction of modern technologies for the production of products with a closed water cycle, etc.).

The research results presented in this article can be the basis for establishing trends changes in the ecological state of the surface waters of the Lower Section of the Ingulets River in time and space, determining the impact of anthropogenic load on ecosystems of water bodies, estimating changes of water quality, informing the public, solving economic and social issues, related to the rational use of natural resources and ensuring environmental protection. The results can be the basis for the analysis of water quality monitoring data on the surface of water bodies of Ukraine, assessing the conditions for the renewal of water resources and obtaining information about the state of water bodies as an important part of the human environment.

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