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Mathematical modelling of process of water quality formation in the Kremenchug reservoir

In terms of active use of water resources for a variety of purposes, including fisheries, drinking, household, agricultural etc., is important to ensure the standard quality of these resources. An important role in the forecasting of surface water quality in a changing environment water management issues is the use of mathematical modelling methods in the solution of this problem.

Here proposes a model of water quality formation in reservoirs taking into account chemical and biological factors. The model is developed on the example of the Kremenchug reservoir. Complex physical, chemical and biological processes in the aquatic environment influences the formation of water quality reservoirs. The income of impurities from external sources, the characteristics of flow and temperature of water influence this process too. Tool that allows us to explore qualitative and quantitative characteristics of the processes of water quality formation is a mathematical model representing the complex kinetics of the transformation of substances involved in the cycle. The most important substances from the point of view of the objectives of water protection are substances for which approved water quality standards. For example, nitrogen compounds included in the composition of bacteria, phytoplankton and zooplankton involved in the nitrogen cycle.

Analysis of the literature showed that a decisive influence on the content of nitrogen-containing substances in surface waters, provide the following factors:

✓ the nitrification process, i.e. a process of consecutive transformation of nitrogen of dissolved organic matter to ammonium nitrogen, nitrite nitrogen and nitrate nitrogen;

✓ the transition nitrogen of suspended organic matter (detritus) in dissolved organic matter;

✓ the presence of feedback between nitrite nitrogen and dissolved organic matter;

✓ the presence of feedback between the content of standardized forms of nitrogen and consumption of intermediate forms;

✓ influence of bacteria on the transformation of nitrogenous substances and on the balance of organic substances;

✓ the role of phytoplankton and zooplankton in nutrient cycle and balance of dissolved oxygen in the aquatic environment;

As input data for the model used data from several years of field observations conducted by the Institute of Hydrobiology Academy of Sciences of Ukraine at the Kremenchug reservoir. In particular, the data on the medium to seasonal concentrations such components of water quality: ammonium nitrogen, nitrate nitrogen and nitrite nitrogen, bacteria Heterotrophs, Nitrosomonas, Nitrobacter, phytoplankton and zooplankton, suspended and dissolved organic matter.

In addition, the model uses data on temperature regime, the magnitude of water runoff, hydrological characteristics of the reservoir and the sources of income-listed component in the Kremenchug reservoir: by river runoff, from bottom sediments, with surface runoff, with subsurface runoff of fertilizers, with industrial and domestic waste waters, with precipitation.

Part of the field data was used to verify the model; the remaining data was used to verify its adequacy.

The basis of the mathematical model is the model of the closed cycle of circulation of nitrogen-containing substances in the water flow, previously presented by the authors in [1]. The proposed model is a modification of the previously developed model for the conditions of reservoirs.

The annual cycle of nitrogen in a reservoir is a complex series of reactions of transformation that has a great influence on the contents of its different forms in water. Mineral nitrogen is assimilated by phytoplankton and bacteria and goes into protein nitrogen. Albumen after dying of organisms is exposed to a mineralization, after that nitrogen of protein substances is allocated in the form of ammonia. Ammonia ni-

trogen is exposed to decomposition by nitrifying bacteria and turns at first to nitrite nitrogen, and then in nitrate nitrogen. However, during the growing period, algae only at high concentrations consume nitrate nitrogen, while ammonium nitrogen is consumed by phytoplankton of 5-10 times more nitrate nitrogen.

The maximum content of mineral forms of nitrogen is observed in the reservoir in the spring, before the flood. This is due to the mineralization of organic matter in the water column and in sediments and their accumulation during the cold period of the year. In the period of spring flood, concentrations of mineral forms of nitrogen begin to decline. Most intensively, this process occurs later, when the activity of phytoplankton and bacteria increases. In addition, the heterogeneity of the plankton development in the reservoir, the circulation of water masses, discharge of sewage leads to uneven distribution of concentrations of mineral nitrogen. With the end of the growing season, algae and the beginning of death of organisms at all trophic levels there is an increased concentration of ammonium nitrogen, nitrite nitrogen and nitrate nitrogen.

Dynamics of organic nitrogen is closely related to the dynamics of aquatic organisms. The concentration of organic nitrogen grows from early spring, reaching maximum values in late summer – early autumn, and then observed for primary reduction.

The distribution of dissolved oxygen in the water column in the spring is almost uniformly. However, there may be a slight stratification, is more pronounced in the shallows where the water warms up sooner and phytoplankton grows faster. During the summer, two opposite processes significantly affect oxygen regime of the reservoir: photosynthesis, in which water is enriched with oxygen, and oxidation of organic substances, leading to decreased oxygen content in water. Summer is especially strongly expressed stratification of the oxygen regime in the reservoirs. The upper layers of water in which there is active photosynthesis, is usually supersaturated with oxygen. In the lower layers, especially for deep reservoirs, there may be a deficiency of oxygen.

In the autumn, the "bloom" of algae leads to a predominance of processes of degradation, which reduces the oxygen content in the water on certain sections and bays. In the late autumn, the stratification is destroyed; the feeding of oxygen over the entire thickness reaches almost 100%.

In the summer the BOD reaches a maximum in the tail of the reservoir, the minimum value of BOD is achieved in the spring. In the autumn, the values of the BOD are reduced, but not all portions of the reservoir.

Seston is an important functional component of aquatic ecosystems. The organic portion of the seston, comprised of detritus and plankton, has a particular effect on the status of aquatic ecosystems.

The part of seston incoming in the Kremenchug reservoir is small compared to the seston produced in the reservoir. The part of seston that enter to the Kremenchug reservoir from without is small compared to the seston generated in the reservoir. Values of seston are very different for the separate areas of the reservoir. Especially sudden fluctuations of values of seston and its components are observed at the bottom of the reservoir, where the most pronounced bloom of freshwater algae. The proportion of detritus in the seston is of the order of 60%, 72% and 67% in spring, summer and autumn respectively. Diatoms and blue green algae, accounting for 65% of the total biomass of plankton in the summer-autumn period, dominate a large part of the vegetation period in the composition of the plankton. In the spring, bacteria dominate the reservoir.

According to the Institute of Hydrobiology Academy of Sciences of Ukraine Kremenchug, water storage refers to the mesotrophic type, so significant parts of the diet of plankton are bacteria. The high content of bacteria Heterotrophs that transform organic matter into mineral forms determines their interaction with dissolved organic matter, but also suspended organic matter.

The above characteristics of the Kremenchug reservoir have been considered in the development of a mathematical model. The model of water quality formation in the reservoir was based on the following scheme of circulation of substances.

Nitrogen dissolved organic matters and suspended organic substances by using bacteria Heterotrophs are transformed into ammonia nitrogen, next with the help of bacteria Nitrosomonas and Nitrobacter in nitrite nitrogen and nitrate nitrogen, respectively. Dying in the life process bacteria enter in suspended organic matter. Ammonia nitrogen and nitrite nitrogen consumed by phytoplankton, which is food for zooplankton. The waste products of zooplankton replenish ammonia nitrogen, dying of phytoplankton and zooplankton are transported into suspended organic matter, part of which goes into dissolved organic matter and the rest using bacteria Heterotrophs go again in ammonia nitrogen. The cycle is completed. Bacteria, phytoplankton and zooplankton consume oxygen for respiration. Dissolved oxygen is consumed in the process of nitrification, which requires aerobic conditions. The process of photosynthesis by phytoplankton increases the dissolved oxygen concentration.

The model accounts dynamics of plankton in the process of the growth of its population in accordance with the principles of kinetics Michaelis - Menten- Mono according to the formula

$$\mu = \frac{\mu_{\max}}{Y} \cdot \frac{N}{K_{SN} + N},$$

where μ - growth rate; $\mu_{\max}$ – maximum growth rate; N is the concentration of nutrients in terms of nitrogen; K_{SN} – constant of half-saturation, Y – economic coefficient, taking into account the recycling of nutrients on the growth of the biomass of the population (in this case bacteria).

The proposed model of formation of water quality in the Kremenchug reservoir is based on the law of conservation of matter in relation to the process of transformation of various forms of nitrogen. It was developed for conditions of steady two-dimensional flows, and taking into account the convective and diffusive transport of substances in the aquatic environment and the influence of water temperature and irradiance on these processes.

A linear operator given bellow describes convective and diffusive transport of substances in the aquatic environment

$$L = u_j \frac{\partial}{\partial x_j} - D \frac{\partial^2}{\partial x_j^2} \quad j = 1, 2,$$

where u_j is averaged by depth flow velocity, D is the longitudinal dispersion coefficient, x_1 and x_2 – coordinate is measured along the length and width of flow respectively.

The effect of water temperature on the magnitude of the main hydro chemical and hydro biological indices is estimated using the temperature coefficients.

$$K_T = \theta^{T-20}; \quad \tilde{K}_T = \frac{T}{20},$$

where T is water temperature in Celsius, θ - experimental constant.

The impact of solar radiation on the growth rate of phytoplankton is estimated using the coefficient of irradiance K_f. The value of this coefficient is equal to the relation of coefficient of solar radiation per season to the average intensity of solar radiation during the completely growing period.

Thus, the model describes the following nitrogen cycle:

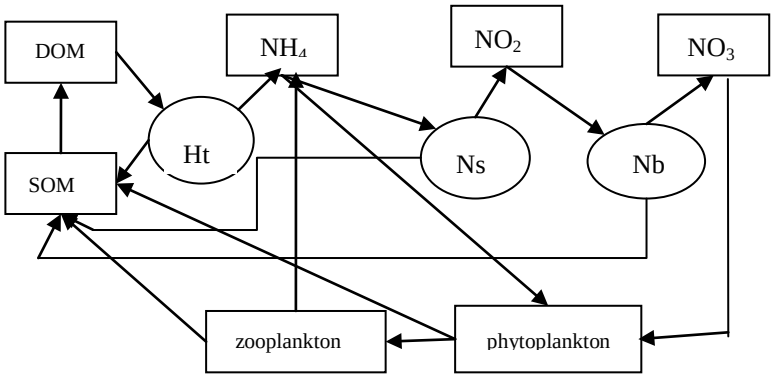
The cycle starts with of the transition of nitrogen, which is part of suspended organic matter (SOM), into dissolved organic matter (DOM). Part of the suspended matter is deposited in sediments, the other part is dissolved. Both processes are evaluated according to the laws of reaction of the first order. Dissolved nitrogen is a substrate for Heterotrophs bacteria, which, as a product of metabolism, are isolated in an aqueous environment, ammonia nitrogen.

In the next stage of cycle (beginning of the nitrification process) bacteria Nitrosomonas participate in the process. They use ammonia nitrogen as a substrate, and excrete nitrite nitrogen as a product metabolism. Nitrobacter bacteria play the main role on the second stage of nitrification. They consume nitrite nitrogen and produce, as a product of the metabolism, nitrate nitrogen. Plankton closes the cycle of transformation and cycling of nitrogen in aquatic ecosystems. Both plankton (phytoplankton and zooplankton) play a dual role. On the one hand, they are living organisms, and the laws of Michaelis - Menten – Mono govern their growth. On the other hand, the phytoplankton is itself a substrate for zooplankton. Phytoplankton uses for

its development two types of substrate – ammonium nitrogen and nitrate nitrogen. At the same time, it is food for zooplankton and it replenishes the suspended organic matter after death.

Zooplankton feeds on phytoplankton, in the process of excretion excretes ammonia nitrogen, when death and defecation restock suspended organic matter. The processes of decay of both types of plankton, defecation and excretion of zooplankton obey the law of the first order. The flow of the products of metabolism of plankton in the form of dissolved organic matter is insignificant in comparison with other elements of the nitrogen cycle, so they can be neglected.

Diagram of the nitrogen cycle given below.



Checking the sensitivity of the proposed model was presented in article [1].

The model uses the following notation:

N_1, N_2, N_3, N_4, N_5 – concentrations (in terms of pure nitrogen) of ammonium nitrogen, of nitrite nitrogen, of nitrate nitrogen, nitrogen of suspended organic matters and nitrogen of dissolved organic matters, respectively.

X_1, X_2, X_3, X_4, X_5 – densities of the biomass of the bacteria Nitrosomonas, Nitrobacter, Heterotroph, phytoplankton and zooplankton, respectively.

K_T *and* $\tilde{K}_T$ are temperatures coefficients.

μ_{max11} is maximum growth rate of Nitrosomonas when they consume ammonium nitrogen, μ_{max22} is maximum growth rate of Nitrobacter when they consume nitrite nitrogen, μ_{max34} is maximum growth rate of Heterotrophs when they consume nitrogen of suspended organic matters, μ_{max35} is maximum growth rate of Heterotrophs when they consume nitrogen of dissolved organic matters, μ_{max41} is maximum growth rate

of phytoplankton when he consumes ammonium nitrogen, μ_{max43} - maximum growth rate of phytoplankton when he consumes nitrate nitrogen.

$\mathbf{Y_{11}}$ is economic coefficient Nitrosomonas when they consume ammonium nitrogen, $\mathbf{Y_{22}}$ is economic coefficient Nitrobacter when they consume nitrogen nitrite, $\mathbf{Y_{35}}$ is economic coefficient Heterotroph when they consume nitrogen of dissolved organic matters.

$\mathbf{k_{S11}}$ is constant of half-saturation for Nitrosomonas when they consume ammonium nitrogen, $\mathbf{k_{S22}}$ is constant of half-saturation for Nitrobacter when they consume nitrogen nitrite, $\mathbf{k_{S35}}$ is constant of half-saturation for Heterotroph when they consume nitrogen of dissolved organic matters, $\mathbf{k_{S41}}$ is constant of half-saturation for phytoplankton when he consumes ammonium nitrogen, $\mathbf{k_{S43}}$ is constant of half-saturation for phytoplankton when he consumes nitrate nitrogen, $\mathbf{k_{S53}}$ is constant of half-saturation for zooplankton when he consumes nitrogen of suspended organic matters, $\mathbf{k_{S54}}$ is constant of half-saturation for zooplankton when he consumes phytoplankton.

$\mathbf{k_{d1}}$, $\mathbf{k_{d2}}$, $\mathbf{k_{d3}}$, $\mathbf{k_{d4}}$, $\mathbf{k_{d5}}$ are mortality rates of Nitrosomonas, Nitrobacter, Heterotroph, phytoplankton and и zooplankton, respectively.

$\mathbf{k_{51}}$ is a coefficient of excretion of zooplankton.

$\mathbf{k_{45}}$ is the coefficient of solubility of the suspended solids.

K_f is the coefficient of irradiance.

f_1, f_2, f_3, f_4, f_5 are the external income of ammonium nitrogen, of nitrite nitrogen, of nitrate nitrogen, of nitrogen of suspended organic matters and of nitrogen of dissolved organic matters, respectively.

In the mathematical model, equations for the substrates are written first, and then the equations for the biomass of bacteria, phytoplankton and zooplankton.

The model equations given below

$$LN_1 = K_T \frac{\mu_{\max 35}}{Y_{35}} \cdot \frac{N_5}{k_{S35} + N_5} X_3 + \tilde{K}_T \cdot k_{51} \cdot X_5 - K_T \frac{\mu_{\max 11}}{Y_{11}} \cdot \frac{N_1}{k_{S11} + N_1} X_1 - \tilde{K}_T \cdot \mu_{\max 11} \frac{N_1}{k_{S11} + N_1} X_1 -$$

$$- K_f \cdot \tilde{K}_T \cdot \mu_{\max 41} \frac{N_1}{k_{S41} + N_1} X_4 + f_1;$$

$$LN_2 = K_T \frac{\mu_{\max 11}}{Y_{11}} \cdot \frac{N_1}{k_{S11} + N_1} \cdot X_1 - K_T \frac{\mu_{\max 22}}{Y_{22}} \cdot \frac{N_2}{k_{S22} + N_2} X_2 - \tilde{K}_T \cdot \mu_{\max 22} \frac{N_2}{k_{S22} + N_2} X_2 + f_2;$$

$$LN_3 = K_T \frac{\mu_{\max 22}}{Y_{22}} \cdot \frac{N_2}{k_{S22} + N_2} \cdot X_2 - K_f \cdot \tilde{K}_T \cdot \mu_{\max 43} \frac{N_3}{k_{S43} + N_3} \cdot X_4 + f_3;$$

$$LN_4 = \tilde{K}_T \cdot k_{d1} \cdot X_1 + \tilde{K}_T \cdot k_{d2} \cdot X_2 + \tilde{K}_T \cdot k_{d3} \cdot X_3 + \tilde{K}_T \cdot k_{d4} \cdot X_4 + \tilde{K}_T \cdot k_{d5} \cdot X_5 - K_T \cdot k_{45} \cdot N_4 + f_6;$$

$$LN_5 = k_{45} \cdot N_4 - K_T \frac{\mu_{\max 35}}{Y_{35}} \cdot \frac{N_5}{k_{S35} + N_5} \cdot X_3 - \tilde{K}_T \cdot \mu_{\max 35} \frac{N_5}{k_{S35} + N_5} \cdot X_3 + f_7;$$

$$LX_1 = \tilde{K}_T \cdot \mu_{\max 11} \cdot \frac{N_1}{k_{S11} + N_1} \cdot X_1 - \tilde{K}_T \cdot k_{d1} \cdot X_1 + f_5;$$

$$LX_2 = \tilde{K}_T \cdot \mu_{\max 22} \cdot \frac{N_2}{k_{S22} + N_2} \cdot X_2 - \tilde{K}_T \cdot k_{d2} \cdot X_2;$$

$$LX_3 = \tilde{K}_T \cdot \mu_{\max 35} \cdot \frac{N_5}{k_{S35} + N_5} \cdot X_3 - \tilde{K}_T \cdot \mu_{\max 53} \cdot \frac{X_3}{k_{S53} + X_3} \cdot X_5 - \tilde{K}_T \cdot k_{d3} X_3 + f_5;$$

The solution of the equations of the model is obtained by numerical methods using MathCAD.

Literature

Nemtsova A. A., Ponomarenko E.G. A structured approach to the construction of models of transformation of substances in the aquatic environment. Materials of XII International research and practice conference, “Advanced science”, - 2016. 30 April – 07 May 2016. Volume 12. Sheffield, UK Science and Education Ltd., 2016. pp. 80 – 94.