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# PREDICTION OF THE HYDROCHEMICAL REGIME OF SURFACE WATER USING SIMULATION MATHEMATICAL MODELLING

## PROGNOZA REŻIMU HYDROCHEMICZNEGO WÓD POWIERZCHNIOWYCH NA PODSTAWIE MODELI MATEMATYCZNYCH

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**Abstract.** Mathematical simulation models of the hydrochemical regime of Velykyi Lyubin pond (Vereshchytsya River basin) and the pond of the Pidhaytsi town (Koropets River basin) have been constructed to clarify the possibilities of using such models in the practice of managing the quality of water resources in small rivers. To evaluate the ecological state of the Vereshchytsya and Koropets river basins – left tributaries of the Dniester – the expedition method was applied, i.e. collecting information on natural conditions and the content of nitrogen compounds (determined directly on-site) as well as $Cl^-$ and $SO_4^{2-}$ ions in water. Information processing was performed by mathematical modelling of the hydrochemical regime of surface waters – calculation models to study the changes in the concentration of biogenic substances and chloride, and sulphate ions in the ponds have been developed. The simulation mathematical models of the hydrochemical regime of surface waters of the ponds were developed for different seasons by a direct construction of the chamber model based on the spatial averaging of the processes and compilation of balance equations. Mathematical models of the change in content of biogenic substances and sulphate, and chloride ions testify to partial purification of waters from pollutants, which is facilitated by the processes taking place within them (sedimentation, sorption–adsorption processes, dissolution).

**Key words:** hydrochemical regime, simulation mathematical models, surface waters, biogenic substances, nitrogen compounds, Velykyi Lyubin and Pidhaytsi ponds, Ukraine.

**Abstrakt.** Opracowano imitacyjne modele matematyczne reżimu hydrochemicznego stawu wielkolubińskiego (dorzecze Wereszczycy) i stawu miasta Podhajcy (dorzecze Koropca) dla wyjaśnienia możliwości wykorzystania takich modeli w praktyce zarządzania jakością zasobów wodnych małych rzeczek. Podczas badania stanu ekologicznego dorzeczy Wereszczycy i Koropca – lewych dopływów Dniestru – wykorzystywano metodę ekspedycyjną – uzyskanie informacji o warunkach środowiskowych, o zawartości związków azotu w wodzie (wyznaczano bezpośrednio na miejscu) i jonów $Cl^-$ i $SO_4^{2-}$. Obróbka danych odbywała się z wykorzystaniem modelowania matematycznego reżimu hydrochemicznego wód powierzchniowych – tworzenie modeli rozliczeniowych dla badania zmiany koncentracji substancji biogenicznych oraz jonów $Cl^-$ i $SO_4^{2-}$ w badanych obiektach. Imitacyjne modele matematyczne reżimu hydrochemicznego wód powierzchniowych stawów wielkolubińskiego i podhajeckiego w różnych porach roku opracowano na podstawie przestrzennego uśrednienia procesów i układania równań bilansowych. Modele matematyczne zmian zawartości substancji biogenicznych oraz jonów $Cl^-$ i $SO_4^{2-}$ świadczą o częściowym oczyszczaniu wód z zanieczyszczeń, czemu sprzyjają procesy sedymentacyjne, sorpcji–adsorpcji oraz rozpuszczania.

**Słowa kluczowe:** reżim hydrochemiczny, imitacyjne modele matematyczne, wody powierzchniowe, substancje biogeniczne, związki azotu, staw wiercholubiński i podhajecki, Ukraina.

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## INTRODUCTION

Contamination of surface and groundwater with nitrogen compounds (ammonium, nitrites and, in particular, nitrates) is a topical problem all over the world. During 2009–2010, in different regions of Ukraine, cases of acute poisoning of children aged under one with water from wells of individual households, in which nitrates were traced in the amounts exceeding permissible concentration values, have been recorded. Nitrates have a negative impact on human body – they influence genetic mechanisms, cause cardio-vascular diseases, and violate metabolism. Toxicity of nitrates results form the chain of transformations: nitrate – nitrite – N-nitroso compounds. The content of nitrates in drinkable water above the level of 50 mg/l causes blood diseases with children and young stock (Horiev *et al*., 1995).

Sewage waters from agricultural fields and animal farms as well as some industrial waters contain many organic compounds of phosphorus. Much nitrogen and phosphorus is available in domestic sewage waters. The increase in content of biogenic elements (especially phosphorus in the form of phosphates) in rivers, lakes and other water reservoirs causes intense development of cyanobacteria as well as some other algae (water reservoir “blooming”). It is accompanied by a rapid reduction in the content of oxygen in water (Vyshnevskyi, 2001).

Natural eutrophication (the process of good plant nutrition) has been in existence for millennia, but the anthropogenic process occurs more quickly, especially in water reservoirs with a slower water exchange – lakes, ponds, water-storage reservoirs, etc. Water eutrophication is the reversible process. In spite of the violation of balance, which results from anthropogenic eutrophication, such water reservoirs can get back to their initial state in case some alien substances do not get there (Burden *et al*., 2004).

This is related to the period of water restoration in nature. It is known that groundwater in the active water reservoir are restored in some 300 years, waters in pond fed by current lakes – in 3.5, river waters – in half a month. And it is of importance that 1 $m^3$ of industrial and domestic sewage contaminates 12–15 $m^3$ of clean water. One kilogram of phosphorus which gets into a water reservoir results in the formation of 100 kg of phytoplankton. Optimal growth of water organisms is traced at the phosphorus concentration of 0.09–1.8 mg/l. A lower content of those elements inhibits algal growth. The results of eutrophication studies show that “water blooming” due to availability of algae appears only when the phosphorus concentration in water exceeds 0.01 mg/l.

The problems of natural water eutrophication are very complex and require scientific analysis, since it is known that moderately eutrophic lakes are more productive and have the best conditions for fishery. In the practice of fishery, lakes and ponds are often artificially fertilized to increase fish productivity, while excessive eutrophication, just the contrary, leads to deterioration of the water quality and fish kill (Manahan, 2001).

## OBJECTS AND METHODS OF RESEARCH

The environmental state of left tributaries of the Dnister (one of Ukraine’s main water arteries), the Vereshchytsya and Koropets’ rivers, which are regulated by ponds, is getting worse. These small rivers constitute the source of the Dnister nutrition and this is why these two rivers were chosen for our study.

Our aim was to build simulation mathematical models of the hydrochemical regime of the Velykyi Lyubin pond (Vereshchytsya River basin) and the pond of the town of Pidhaytsi (Koropets’ River basin) (Fig. 1) to clarify the possibilities of using such models in the practice of water resources quality management of small rivers.

To study the ecological state of the Vereshchytsya and Koropets’ river basins, the expedition method was applied. It uses information about natural conditions and the content of nitrogen compounds in water (determined directly on-site) as well as $Cl^-$ and $SO_4^{2-}$ ions. Information processing was performed by mathematical modelling of the hydrochemical regime of surface waters – calculation models to study the change in the concentration of biogenic substances and chloride and sulphate ions in the pounds were developed and their environmental condition was predicted.

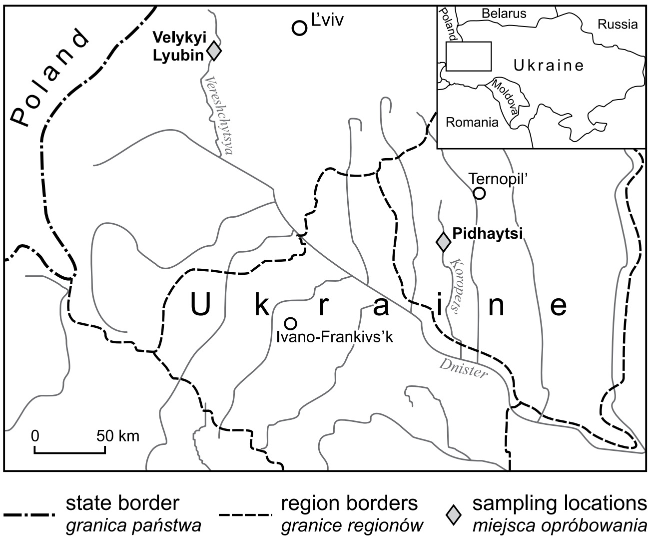


**Fig. 1. Location map of the research area**

Lokalizacja terenu badań

## RESULTS

The development of the simulation mathematical model of the hydrochemical regime of surface waters of the Velykyi Lyubin and Pidhaytsi ponds was carried out by a direct construction of the chamber model based on the spatial averaging of processes and compilation of balance equations (Lavryk, 2002). Hydrochemical regime of surface waters is a natural historical process of change in the condition and properties of waters in time and within the fixed space, which undergoes under the influence of the whole integrity of certain interacting and permanently changing natural and artificial factors.

To determine the dynamics of salt concentration in the lake, in case where initial concentration of salts in the lake is $c_0$, and the level of water in it is not changed ($q_1 = q_2$), we will use the following formula:

$$c^*_{pond}(t) = k + (1-k)\exp\left(-\left(\frac{1+\alpha^j\tau_0}{\tau_0}\right)t\right),$$

where:

$c^*_{pond} = \frac{c_{pond}}{c_0}$;

$k = \frac{c^*_\gamma}{c_0}$ – non-dimensional (aggregate) values determining the concentration of salts in the pond through initial concentration $c_0$;

$k$ – factors of dilution or mixing;

$\alpha^{ij}$ – sedimentation speed constant;

$t$ – time in days. The time of complete water restoration in the lake $\tau_0$, which characterizes water exchange on condition of absence of mixing, was determined by the following formula:

$$\tau_0 = \frac{W_0}{q^0 + q_f + q_{prec} - q_{evap}},$$

where:

$W_0$ – water scope in the pond at the initial moment of time $t = t_0$;

$q^0$ – flow (spending) of water from the river into the pond;

$q_f$ – filtration loss of underground waters;

$q_{prec}$ – amount (flow) of precipitation falling onto the water surface of the pond;

$q_{evap}$ – value (flow) of evaporation from the pond surface.

Due to insufficiency of information, the impact of chemical, biological or radioactive disintegration is not taken into account. Sedimentation speed constant $\alpha^j$ was determined on an iterated basis in the course of modelling, coordinating values of the model and actual concentrations.

To assess the changes in the hydrochemical regime, the results of determination of the concentration of biogenic substances and sulphate and chloride ions were used. As the result, mathematical models for different seasons were developed (Figs. 2–3).

According to our model, the increase in the content of biogenic substances in the pond of the town of Velykyi Lyubin takes place during the summer and autumn periods. To be more specific, the content of nitrate ions increases significantly in the period from August to November, the content of phosphate, chloride and sulphate ions remains relatively stable with the upward tendency for the content of sulphate ions in June and the content of phosphate ions in November. The pond in the town of Pidhaytsi is characterized by elevated contents of nitrite, nitrate and phosphate ions in the period from August to September, and chloride and sulphate ions from August to November. Such a distribution is caused by the specificity of economic activity within a certain territory, viz. availability of pastures (livestock waste) and farms (the use of mineral and organic fertilizers), growth of fish in ponds. Substantial amounts of nitrite, nitrate and phosphate ions are brought by run-off from the adjacent territories during intense precipitation in summer and autumn months.

## CONCLUSIONS

Mathematical models of the content of biogenic substances and sulphate, and chloride ions prove partial purification of pond waters from pollutants. The processes that take place in the studied ponds (sedimentation, sorption–adsorption process, dissolution) also contribute to that. This has a positive impact on the quality indices of surface waters of the hydrochemical systems under research. Such systems must be under permanent control, since a considerable increase in the content of, for instance, biogenic substances can lead to intense breeding of water organisms, and, as the result, eutrophication in the water reservoir is accelerated.

The development of mathematical models of the hydrochemical regime of surface waters enables to forecast the changes in the condition and properties of waters in time and within some specific water reservoirs as well as to take steps to prevent deterioration of the environmental condition of surface waters, and thus, groundwater.

To optimize the condition of water ecosystems, it is recommended to use the methods of mathematical modelling on a wider basis, as they improve reliability of determination of both the very fact of contamination, its scope and origin. The results of mathematical modelling enable to assess the advantages and disadvantages of each of the alternative solutions associated with the protection of water resources within the framework of implementation of environmental programs relating to ensuring the reproducible development, introduction of programs and projects of local, regional and national importance.

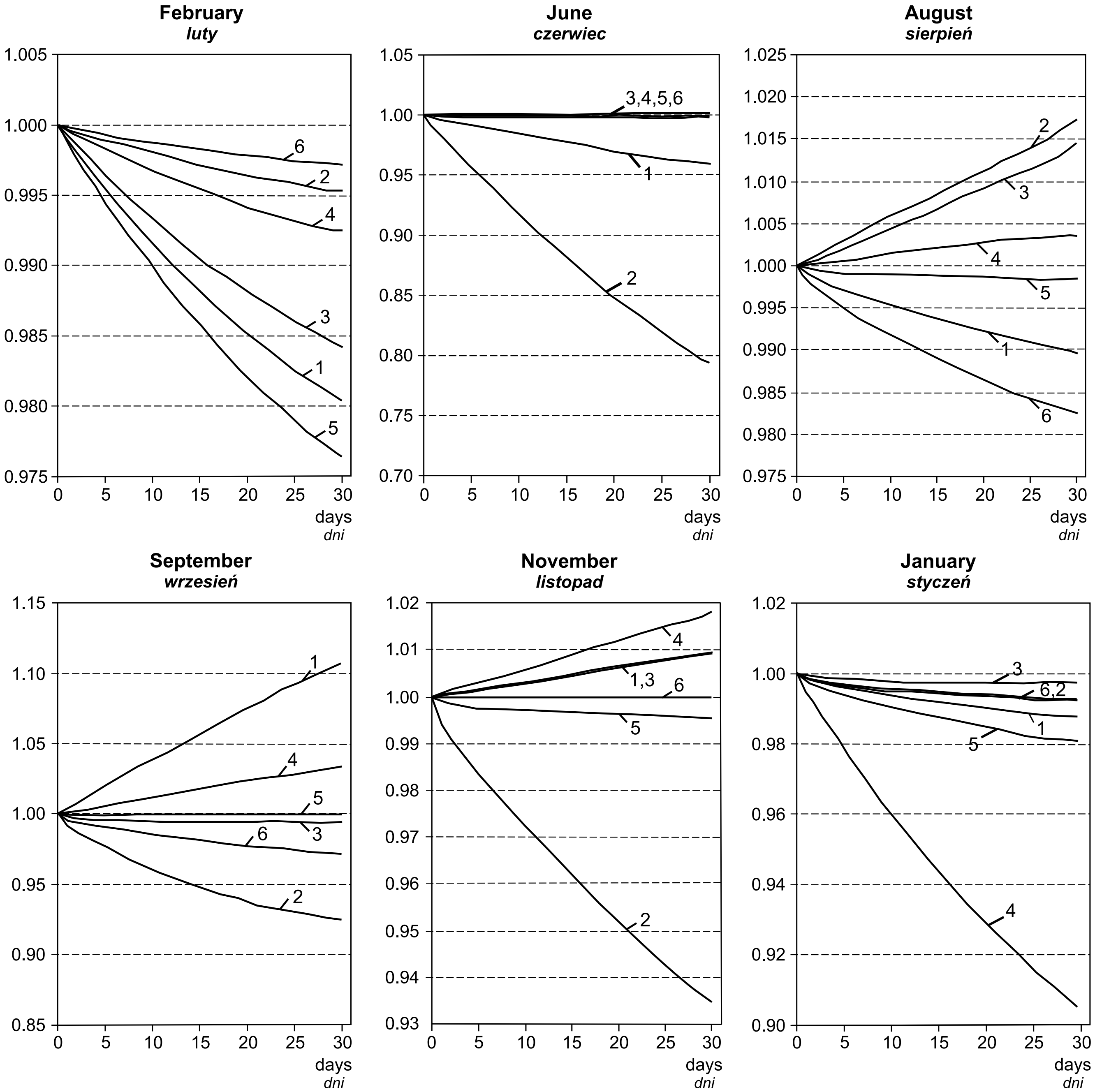


**Fig. 2. Mathematical models of hydrochemical regime of waters in Velykyi Lyubin pond (Y axis shows the change of aggregate concentration of biogenic substances and $Cl^-$ and $SO_4^{2-}$ ions with time; X axis shows days): 1 – $NH_4^+$; 2 – $NO_2^-$; 3 – $NO_3^-$; 4 – $PO_4^{3-}$; 5 – $Cl^-$; 6 – $SO_4^{2-}$**

Modele matematyczne reżimu hydrochemicznego wód w zbiorniku wielkolubińskim (na osi Y zmiany stężeń substancji biogenicznych oraz jonów $Cl^-$ i $SO_4^{2-}$ w czasie; oś X liczba dni): 1 – $NH_4^+$; 2 – $NO_2^-$; 3 – $NO_3^-$; 4 – $PO_4^{3-}$; 5 – $Cl^-$; 6 – $SO_4^{2-}$

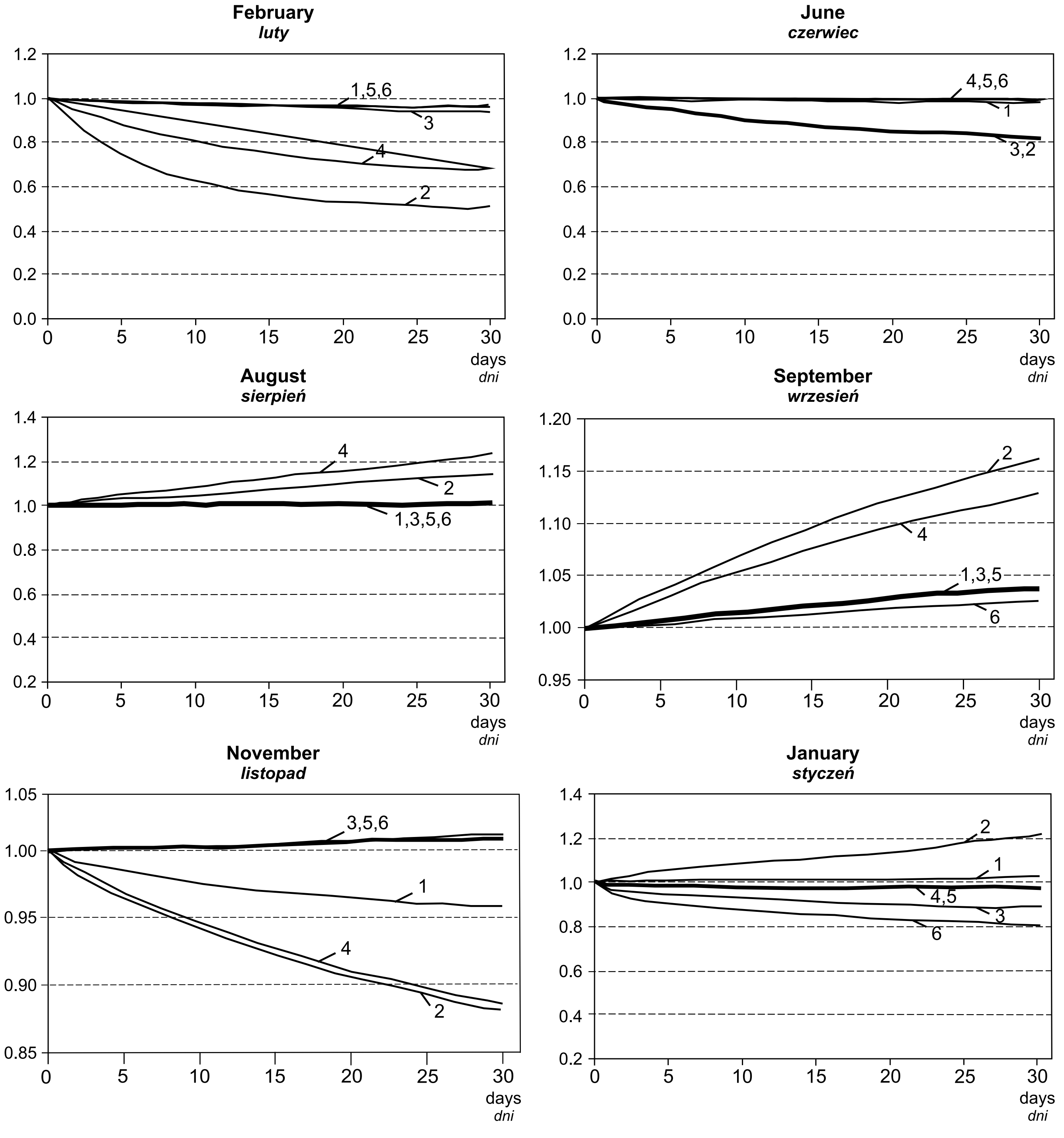


**Fig. 3. Mathematical models of hydrochemical regime of waters of Pidhaytsi pond (Y axis shows the change of aggregate concentration of biogenic substances and $Cl^-$ and $SO_4^{2-}$ ions with time; X axis shows days); 1 – $NH_4^+$; 2 – $NO_2^-$; 3 – $NO_3^-$; 4 – $PO_4^{3-}$; 5 – $Cl^-$; 6 – $SO_4^{2-}$**

Modele matematyczne rezimu hydrochemicznego wód w zbiorniku podhajeckim (na osi Y zmiany stężeń substancji biogenicznych oraz jonów $Cl^-$ i $SO_4^{2-}$ w czasie; oś X liczba dni); 1 – $NH_4^+$; 2 – $NO_2^-$; 3 – $NO_3^-$; 4 – $PO_4^{3-}$; 5 – $Cl^-$; 6 – $SO_4^{2-}$

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