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Mathematical modelling of the pollution processes of the Southern Bug River by nitrogen-containing compounds

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Abstract. Critical ecological state of the Southern Bug River, caused by intensive pollution with nitrogen-containing compounds, requires the implementation of reliable mathematical forecasting tools to mitigate the effects of eutrophication and achieve the objectives of national water resources management strategies. The study aimed to mathematically model the processes of transport and transformation of nitrogen-containing compounds in the Southern Bug River system to quantitatively assess the spatio-temporal dynamics of pollution and provide a scientific basis for environmental protection measures. For the mathematical modelling, a system of differential equations based on one- and two-dimensional advection-dispersion-reaction models was applied, the numerical solution of which was conducted using the operator splitting method. Developed a model that integrated the three key nitrogen components and accounted for the mechanisms of advection, dispersion and biochemical transformations. The model described the processes of nitrification and denitrification in detail, incorporating temperature and dissolved oxygen concentration according to the Michaelis-Menten kinetics. Modelling was conducted to assess the impact of ammonium nitrogen pollution, using the example of discharges from municipal wastewater treatment plants in the upper reaches. The verification results demonstrated the model's ability to reproduce the spatial reduction in pollutant levels due to natural self-purification processes. The model identified the formation of a "nitrite peak", which is spatially shifted downstream relative to the maximum ammonium concentrations. High levels of toxic nitrites persist at distances of up to 15 km from the source of pollution. A scenario analysis has shown that the immediate implementation of tertiary treatment at the most significant facilities is a priority measure for restoring the river's oxygen regime. If the river's water flow decreases by 40% of the normal low-water level, a catastrophic increase in the concentrations of nitrogen-containing compounds and oxygen depletion is expected across significant sections of the river channel, provided that current discharge volumes remain unchanged. The model developed serves as a tool for optimising management decisions within the framework of the Southern Bug River Basin Management Plan and created a comprehensive environmental monitoring system to ensure the region's sustainable development

Keywords: water; environmental safety; environmental monitoring; ammonium ions; nitrite ions; nitrate ions; nitrification; denitrification

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Introduction

The Southern Bug River is one of the most substantial waterways, yet it is subject to critical anthropogenic pressure due to the discharge of inadequately treated domestic and industrial wastewater. This causes intense pollution by nitrogen-containing compounds (NCCs), in particular ammonium, nitrite and nitrate nitrogen, leading to widespread eutrophication, oxygen depletion and severe toxic-hypoxic stress on aquatic ecosystems. The situation is significantly exacerbated by the high degree of river channel regulation, which substantially slows the flow and inhibits the water body's natural self-purification mechanisms. To overcome this large-scale environmental crisis and achieve the objectives of national water resource management strategies, it is not enough merely to note that sanitary standards are being exceeded many times over. There is a need to develop and implement reliable predictive mathematical tools that will not only quantitatively assess the current extent of pollution, but also reliably predict the spatio-temporal dynamics of pollutant spread and scientifically substantiate the effectiveness of priority infrastructure-based environmental protection measures.

M.T. Ejigu (2021) conducted a comprehensive review of current approaches to modelling water quality in open water bodies. The study analysed the evolution of mathematical models from simple empirical relationships to complex dynamic systems that consider multi-component biochemical reactions. According to the researcher, the choice of the optimal structure for a mathematical model depends critically on the availability of high-quality monitoring data and the specific characteristics of the hydrological regime of a particular water body. I. El Arabi *et al.* (2022) investigated the possibilities of numerical modelling using the advection-dispersion-reaction (ADR) equation for a one-dimensional contaminant transport problem. The finite difference method and the operator splitting method were successfully applied to optimise the computational process. This mathematical approach ensures high stability and accuracy of the solution when modelling the spatial distribution of pollutants in media with saturated porosity and in river flows.

According to H. Qiu *et al.* (2023), an integrated system was developed for spatial modelling of nitrogen transport and transformation across an entire catchment. The study addressed the complex interrelationship between hydrological cycles and biogeochemical processes of nutrient transformation. Study determined that accurately modelling the spatial heterogeneity of pollution sources is a key factor in improving the overall predictive capability of catchment-scale environmental models. E.G. Tsega (2024) developed numerical solutions for two-dimensional non-linear, non-stationary advection-dispersion-reaction equations with variable coefficients. The influence of transverse and longitudinal dispersion on the formation of pollution plumes under variable hydrodynamic conditions was investigated. The results of the study demonstrated that the use of two-dimensional models is essential for an adequate description of areas near local point sources, where the classical one-dimensional approximation yields significant errors.

H. Yu *et al.* (2024) analysed the mechanisms of nitrate formation in biochemical treatment processes and the influence of operating conditions on these reactions. The kinetics of ANN transformations under the action of specific microbial communities were examined. Temperature and dissolved oxygen concentration are the main limiting factors that directly determine the rate and extent of nitrification and denitrification reactions in aquatic ecosystems. According to researchers X. Yan *et al.* (2025), effective water quality management requires a combination of engineering technologies for nitrogen removal with comprehensive catchment area management. The synergistic effect of modernising urban wastewater treatment plants and implementing environmental protection practices in agriculture was assessed. Only such an integrated approach can ensure a sustainable reduction in the trophic status of water bodies and ultimately prevent their further ecological degradation.

A. Pukish *et al.* (2024) conducted mathematical modelling of the processes of groundwater aquifer contamination resulting from mineral extraction. Predictive models of contaminant migration in porous media were developed, taking complex hydrogeological conditions into detailed account. The use of numerical modelling methods made it possible to identify, with a high degree of accuracy, the areas of greatest environmental risk and to optimise preventive measures for the protection of water resources. The impact of phytoremediation technologies on water quality was analysed, and the potential of such systems for locally reducing the concentration of biogenic elements was assessed. The implementation of such nature-based solutions is an effective tool for improving the environmental condition of local areas, but it requires integration with broader catchment-level strategies.

Despite the considerable number of scientific papers devoted to modelling water quality and biogeochemical nitrogen cycles, an integrated combination of one-dimensional and two-dimensional transient models specifically tailored to the conditions of highly regulated rivers with extreme levels of point source pollution remains insufficiently studied. In particular, the synergistic influence of oxygen limitation, seasonal temperature fluctuations and the retention properties of bottom sediments on the kinetics of ANN transformation at the scale of large river basins in Ukraine remains insufficiently studied and formalised. Therefore, the study aimed to mathematically model the processes of ANN transport and transformation in the Southern Bug River system.

Materials and Methods

Water quality modelling is substantial for assessing the ecological status of the Southern Bug River, forecasting the spread of pollution and developing effective water management measures. Modelling of ANN – ammonium (NH_4^+), nitrites (NO_2^-) and nitrates (NO_3^-) – was prioritised as excessive concentrations of these are key indicators of chemical pollution and cause eutrophication of water bodies. The transport and transformation of dissolved substances in river systems have been most accurately described by the one-dimensional ADR equation (Bakken *et al.*, 2012; Genuchten *et al.*, 2013; Shang *et al.*, 2021; Kumar *et al.*, 2022; Qiu *et al.*, 2023). This model is the standard for hydroecological studies, as it encompasses three fundamental mass transport processes. Process of advection is the transport of dissolved substances with the main water flow at a rate of V. For a river such as the Southern Bug, advection is the dominant transport mechanism.

The dispersion process is the spread of a pollutant from areas of high concentration to areas of low concentration. The dispersion coefficient (D_L) is not a constant value and depends on hydraulic parameters; its value may increase significantly in reservoirs compared with river channel sections. The reaction process refers to changes in the concentration of a compound resulting from biological (e.g. nitrification, denitrification) and abiotic (sorption/sedimentation) processes. As biochemical processes in the river, in particular the rate of denitrification, exhibited high diurnal and seasonal variability, the use of a transient equation was necessary (Yao & Peng, 2017; Sridharan & Hein, 2019; Gordillo *et al.*, 2020). The ADR system for the river section with constant hydraulic parameters (A, V, D_L) was as follows:

$$\frac{\partial C_i}{\partial t} + V\frac{\partial C_i}{\partial x} = D_L\frac{\partial^2 C_i}{\partial x^2} + R_i + S_i, \quad (1)$$

where C_i – concentration of i-th compound; t – time; x – longitude along the river; D_L – coefficient of longitudinal hydrodynamic dispersion; V – average flow speed; R_i – rate of inflow and outflow of i-th compound through reaction; S_i – rate of inflow from distributed and point sources/discharges.

Advection ($V\frac{\partial C_i}{\partial x}$) described the transport of compounds along the x-axis with the main flow at an average velocity of V. Dispersion ($D_L\frac{\partial^2 C_i}{\partial x^2}$) incorporated the longitudinal spread of the substance (mixing) from areas of high concentration to areas of low concentration. The coefficient of longitudinal hydrodynamic dispersion (D_L) was critical in areas with rapidly changing hydraulic conditions, particularly in reservoirs. To accurately model the nitrogen cycle in the Southern Bug, the ADR model included three coupled equations for ammonium, nitrites and nitrates, as the products of one reaction act as reactants for the next.

Ammonium () was a cation capable of being sorbed onto river sediments, which slowed its migration in the aquatic environment. Therefore, its transport equation had to be modified by introducing a retardation factor (R_{NH_4})):

$$R_{NH_4}\frac{\partial C_{NH_4}}{\partial t} = D_L\frac{\partial^2 C_{NH_4}}{\partial x^2} - V\frac{\partial C_{NH_4}}{\partial x} - R_{N1} - R_{Sor} + S_{NH_4}, \quad (2)$$

where R_{NH_4} – retardation factor (typical range 1.1 – 2.5); R_{N1} – use rate NH_4^+ phase I nitrification (conversion to NO_2^-); R_{Sor} – loss rate NH_4^+ due to absorption and sedimentation; S_{NH_4} – ammonium inputs (mainly from point sources, such as municipal wastewater).

Nitrites (NO_2^-) were an intermediate, highly reactive product of nitrification. The nitrite balance was determined by their formation from ammonium (R_{N1}) and their consumption in the formation of nitrates (R_{N2}):

$$\frac{\partial C_{NO_2}}{\partial t} = D_L\frac{\partial^2 C_{NO_2}}{\partial x^2} - V\frac{\partial C_{NO_2}}{\partial x} + R_{N1} - R_{N2}, \quad (3)$$

where R_{N1} – increase of NO_2^- from nitrification (phase I); R_{N2} – decrease of NO_2^- from nitrification (phase II).

Nitrates (NO_3^-) were end products of oxidation:

$$\frac{\partial C_{NO_3}}{\partial t} = D_L\frac{\partial^2 C_{NO_3}}{\partial x^2} - V\frac{\partial C_{NO_3}}{\partial x} + R_{N2} - R_D - R_{Alg} + S_{NO_3}, \quad (4)$$

where R_{N2} – increase of NO_3^- from nitrification (phase II); R_D – decrease of NO_3^- through denitrification (the anaerobic conversion to gaseous nitrogen, which occurs mainly in sediments); R_{Alg} – consumption rate of NO_3^- by phytoplankton and algae; S_{NO_3}) – nitrate inflow.

Furthermore, it was necessary to incorporate correction factors into the mathematical model to account for the influence of temperature (T) and dissolved oxygen (DO) on biochemical processes. The water temperature in the river, in turn, was influenced by several natural and anthropogenic factors (Boychenko *et al.*, 2017). A decrease in ambient temperature was a critical factor limiting the functional capacity of denitrifying microflora (Liao *et al.*, 2018; Nevorski & Marcarelli, 2022). This reduced the efficiency of nitrogen compound removal and led to ammonium nitrogen and total nitrogen levels in the effluent exceeding regulatory limits during the cold season (Gao *et al.*, 2024; Ibarra *et al.*, 2024).

Temperature correction was conducted as follows: the kinetic rate constant k_i of the chemical reaction was corrected using a modified form of the Arrhenius equation (Davidson *et al.*, 2012; Gomolka *et al.*, 2022):

$$k_i(T) = k_{i,20} \cdot \Theta^{(T-20)}, \quad (5)$$

where i – index $N1$ for phase I of nitrification, $N2$ for phase II of nitrification, D for denitrification; $k_{i,20}$ – kinetic rate constant of a chemical reaction, determined at 20 °C (for nitrification, typical range is 0.1-0.5 day^{-1}, for denitrification); T – temperature (°C); Θ – temperature coefficient (typical values are 1.080 for the nitrification reaction and 1.045 for denitrification reaction).

Given the significant ammonium pollution in the Southern Bug, which caused oxygen deficiency, oxygen limitation was the key factor regulating the rate of purification. Since nitrification is an aerobic process, modelled as a first-order reaction limited by oxygen concentration, the effect of dissolved oxygen was considered as follows:

$$R_{N1} = k_{N1}(T) \cdot C_{NH_4}) \cdot f_{nit}(\mathrm{DO}); \quad (6)$$

$$R_{N2} = k_{N2}(T) \cdot C_{NO_2}) \cdot f_{nit}(\mathrm{DO}). \quad (7)$$

According to the Michaelis-Menten equation (Davidson *et al.*, 2012), a coefficient that addresses the effect of oxygen on the rate of nitrification f_{nit} (DO), was as follows:

$$f_{nit}(\text{DO}) = \frac{\text{DO}}{k_{\text{OA}}+\text{DO}}, \tag{8}$$

where DO – concentration of dissolved oxygen in water (mg/l); k_{OA} – oxygen half-saturation constant (Michaelis constant) for nitrifying bacteria (mg/l).

Parameter k_{OA} indicated the oxygen level at which the rate of nitrification is halved. In river models, the typical value of k_{OA} is 0.5-2.0 mg/l. If the concentration of dissolved oxygen in the water fell below 0.5 mg/l, nitrification practically ceased, as the nitrifying microorganisms lost the competition for oxygen to other heterotrophs.

The equation for dissolved oxygen (DO) concentration addressed its consumption during nitrification and natural replenishment via surface re-aeration:

$$\frac{\partial \text{DO}}{\partial t} = D_L \frac{\partial^2 \text{DO}}{\partial x^2} - V\frac{\text{DO}}{\partial x} - R_{nit,\text{O}_2} + R_{reaer}, \tag{9}$$

where $R_{nit,\,O2}$ – oxygen consumption for nitrification $R(nit, O_2) = YN \cdot (R_{N1} + R_{N2})$; Y_N – stoichiometric oxygen consumption coefficient; R_{reaer} – reaction rate, describing the process of oxygen diffusion from the atmosphere into water when a deficiency arises $R_{reaer} = k_a \cdot (\text{DO}_{\text{sat}} - \text{DO})$; – coefficient that depends on the flow velocity V and depth H; DO_{sat} – oxygen saturation concentration at a given temperature T. Since denitrification was a heterogeneous anaerobic process occurring at the "water-bottom sediment" interface, the rate of denitrification was inversely proportional to the depth of the river. To convert to volumetric modelling parameters, the areal coefficient $(k_{D,\,A})$ (T) was converted to spatial $(k_D(T))$ by dividing by the average depth of the river (H):

$$k_D(T) = \frac{k_{D,A}(T)}{H}, \tag{10}$$

where $k_{D,\,A}(T)$ – areal denitrification rate (per unit of seabed area); typical range of values 0.01 – 0.5 rN $\cdot$ day^{-1} $\cdot$ m^{-2}; H – river depth (m).

A range of areal velocity was selected to model the denitrification process from 0.05 to 0.2 gN $\cdot$ day^{-1} $\cdot$ m^{-2}, which corresponded to the average values for mesotrophic rivers in the temperate zone. In silty sediments rich in organic matter, the velocity was 5-10 times higher than in sandy sediments (Wenjin & Ruijie, 2008). The conversion to specific volumetric flow rate was conducted based on hydromorphometric characteristics of the river channel, which addressed the scaling effect for moving from local bed processes to the overall nitrogen balance in the flow.

Covering the effect of dissolved oxygen on the denitrification process:

$$R_D = \text{k}_\text{D}(T) \cdot C_{NO3}) \cdot \text{f}_{\text{den}}\text{DO}), \tag{11}$$

where $k_D(T)$ – volumetric denitrification rate (in the water column); C_{NO_3} – nitrate concentration; f_{den} (DO) – coefficient that incorporates the effect of oxygen on the rate of denitrification.

In contrast to nitrification, where oxygen activates the process, oxygen acted as an inhibitor in denitrification (García-Ruiz *et al.*, 1998; Bakken *et al.*, 2012). The inverse Michaelis-Menten function was used (Davidson *et al.*, 2012):

$$f_{den}(\text{DO}) = \frac{k_{in}}{k_{in}+DO}, \tag{12}$$

where k_{in} – inhibition constant, typical range 0.1 – 0.5 mg/l; DO – concentration of dissolved oxygen in water (mg/l).

As denitrification is a facultative anaerobic process, its rate in the model was controlled by a kinetic inhibition term. The use of the constant k_{in} made it possible to formalise the switch in microbial metabolism from nitrate respiration to aerobic respiration as the concentration of dissolved oxygen increased. This reflected the actual dynamics of the process, which was localised predominantly in anoxic microzones of bottom sediments, where oxygen diffusion is limited. In the river, the concentration of dissolved oxygen was usually sufficiently high in the water column, but low in the silt. The regulation of the Southern Bug River basin resulted in the accumulation of silty bottom sediments in reservoirs, ponds and other sections of the river with low flow velocities. In these sections, within the silt layer with a low concentration of dissolved oxygen, the process of denitrification took place effectively.

As an analytical solution to the system of differential equations (2-4) was not possible due to the variability of the hydraulic parameters and the non-linearity of the reaction terms, it was necessary to apply numerical methods (Pérez Guerrero *et al.*, 2009; Oñate *et al.*, 2017). The most effective approach for modelling transport in rivers was the operator splitting method, which divided the full ADR equation into separate phases that were solved sequentially. To ensure the stability of the model, an implicit finite difference scheme was used for the dispersion term. This resulted in a system of linear algebraic equations with a tridiagonal matrix, which could be efficiently solved using the Tridiagonal Matrix Algorithm. The Southern Bug catchment was a hydrographically complex system, characterised by considerable length and a high degree of regulation. The high degree of regulation significantly slowed the flow, which impeded natural self-purification processes and created a cumulative effect of pollution. This spatial heterogeneity necessitated hydraulic segmentation (discretisation), which treated parameters as constant within each segment (Alexander *et al.*, 2009). Current European methodology involves the identification of surface water bodies (SWBs), which serve as the basic unit for modelling. In the Southern Bug catchment, 1,090 SWBs were identified, including 375 river bodies, 692 potentially heavily modified bodies and 22 artificial bodies.

The segmentation, which is critical to the model, addressed hydraulic zones such as point discharge zones, channel sections and reservoir zones. The flow velocity (V) and cross-sectional area (A) were determined by the following factors. In typical channel sections, the flow velocity (V) varied within the range 0.2-0.6 m/s. The average depth (H) in the channel segments was approximately 1.5-3.0 m. In reservoirs, due to impoundment, the average velocity decreased significantly, which increased the water residence time. This had a direct impact on transformation and self-purification processes. The longitudinal dispersion coefficient (D_L) described turbulent mixing and was critically dependent on the channel morphology. In sections of the river channel with higher flow velocity and shallower depths, the longitudinal dispersion coefficient was lower, in the range of 10-50 m²/s.

Simulations for a one-dimensional model based on the ADR equation were conducted on a section of the Southern Bug River stretching from the village of Kopystyn to the village of Nova Syniavka. The average morphometric parameters of the river channel for the study section were taken from the Southern Bug River Basin Management Plan for 2025-2030 (Afanasiev *et al.*, 2024) and the study by V.K. Khilchevskyi *et al.* (2009). The average channel width varied from 10 to 15 m at the start of the section (near Kopystyn), gradually widening to 20-30 m closer to Nova Syniavka. In some sections, the river's width locally increased to 50 m. The average channel depth ranged from 0.5 to 1.5 metres. At the start of the section (near the village of Kopystyn, slightly downstream of Khmelnytskyi), the average annual water flow was approximately 2.5-3.0 m³/s (during periods of summer low water, it could fall to 0.8 m³/s). Closer to the village of Nova Syniavka, the water flow increased and averaged 5-8 m³/s. The longitudinal dispersion coefficient is 10-50 m²/s according to the study (Chapra, 1997). Pollution indicators for the studied section of the Southern Bug River in the ANN were taken from publicly available data from the State Agency for Water Resources of Ukraine as of 2018. For subsequent years of observation, pollution data for this section are provided only partially; in particular, data for the village of Kopystyn are missing from 2019 onwards. Input parameters for the mathematical modelling of the processes of pollution of a river segment by NCCs, based on the ADR equation, are given in Table 1. The coefficients for the ADR equation were selected following G.L. Bowie *et al.* (1985).

Table 1. Input data for the mathematical model based on the ADR equation

Physical quantity	Variable	Value	Units of measurement	Range of variation in the study area
Length of the river section to be modelled	L	80	km	-
Average flow velocity	V	0.5	m/s	0.2-0.6
Coefficient of longitudinal dispersion	D_L	20	m²/s	10-50
Retardation factor for ammonium	R_{NH4}	2	-	1.1-2.5
Average depth of the river	H	1	m	0.5-1.5
Water temperature (for September 2018)	T	16	°C	11-20
Concentration of dissolved oxygen	DO	5	mg/dm³	-
Phase I nitrification rate constant	$k_{N1,20}$	0.5	day^{-1}	0.1-0.5
Phase II nitrification constant	$k_{N2,20}$	0.5	day^{-1}	0.1-0.5
Area-specific denitrification rate	$k_{D,A,20}$	0.01	$gN \cdot day^{-1} \cdot m^{-2}$	0.01-0.5
Oxygen half-saturation constant for nitrification	k_{OA}	1.0	mg/l	0.5-2.0
Inhibition constant for denitrification	k_{in}	0.25	mg/l	0.1-0.5
Reaction coefficient	k_a	0.3	day^{-1}	0.2-0.8
Number of spatial nodes (segments).	N_x	800	-	-
Maximum ammonium concentration	C_{source_NH4}	6	mg/dm³	-

Source: compiled by the authors based on G.L. Bowie *et al.* (1985)

Due to the significant spatial and temporal variability of hydraulic parameters and the non-linearity of kinetic processes, it is impossible to determine all parameters precisely by analytical means. Therefore, to obtain a working model suitable for forecasting, it was necessary to conduct a calibration and verification stage. In the first stage, approximate values of hydraulic (D_L) and kinetic (k_i) parameters, obtained from the literature for similar river systems (Bowie *et al.*, 1985), were applied. The exact coordinates and characteristics of point source discharges (PSD) were modelled as internal boundary conditions. In the subsequent modelling stages, the unknown parameters were calibrated until the modelled profiles of ANN concentrations corresponded as closely as possible to the actual monitoring data, particularly in critical zones. Following the requirements for modelling the spatio-temporal distribution of pollution sources as internal boundary conditions, it is necessary to incorporate that the ADR model must include the S_i term – the net inflow rate of the i compound from point sources of discharge.

In the context of the Southern Bug River, sources of pollution had a significant impact on the quality of surface waters. The modelling accounted for point sources that generate maximum peak loads. Point sources, primarily discharges of inadequately treated domestic sewage, were modelled as internal boundary conditions (S_{NH_4}), introducing a high mass flow $F_S = Q_S \cdot C_S$ at a specific coordinate x_S. Monitoring data indicated that the greatest load is concentrated in the upper reaches of the river downstream of Khmelnytskyi. Although the critical zone is in the upper reaches, other large cities further downstream are also significant sources of pollution. The one-dimensional ADR model was transient (time-dependent), as municipal wastewater discharges can vary over the course of a day, a week or depending on the hydrological situation (El Arabi *et al.*, 2022). Point sources were characterised by high concentrations of ammonium nitrogen and organic compounds (high BOD_5), leading to oxygen deficiency, which in turn limited the rate of nitrification.

Given the considerable length of the Southern Bug River and the assumption of rapid transverse mixing within the river channel, most hydroecological studies have traditionally used one-dimensional (1D) models. However, to model the spread of pollution from point sources and account for lateral dispersion in the discharge zone, it is advisable to use a two-dimensional (2D) model (a stationary plane-flow problem) (Hamdi, 2007; Cueto-Felgueroso *et al.*, 2019; Hwang, 2021). In this case, equations (2-4) were modified by adding terms that account for lateral dispersion and removing terms that account for time variation. Modelling for the 2D ADR equations was conducted on a section of the Southern Bug River from the village of Kopystyn to the drinking water intake in the city of Vinnytsia. According to the Southern Bug River Basin Management Plan (Afanasiev *et al.*, 2024), the average channel width ranges from 15-25 m in the Kopystyn area to 40-80 m near the city of Vinnytsia. The average depth is 2-3 m. The average annual water flow near the village of Kopystyn (the start of the section) is approximately 2.5-3.5 m³/s (during the summer low-water period, this may decrease to 0.8-1.5 m³/s), near the town of Khmilnyk – 10-14 m³/s, and near the city of Vinnytsia – 25-30 m³/s (10-12 m³/s during the summer low-water period). The longitudinal dispersion coefficient is 5-25 m²/s according to the study (Chapra, 1997). Pollution indicators for the studied section of the Southern Bug River were taken from publicly available data from the State Agency for Water Resources of Ukraine as of 2018, which was used for a comparison of the pollutant concentrations with the modelling results. It is not possible to use pollution data for the site after the specified date, as the figures for these monitoring points are no longer officially published, although instances of pollution continued to be recorded by civil society organisations.

The system described the mass balance for three related nitrogen components: ammonium (C_{NH_4}), nitrites (C_{NO_2}) and nitrates (C_{NO_3}). In the 2D steady-state form, the ADR equation, assuming constant hydraulic parameters on segment (V, D_L, D_T), is:

$$D_L \frac{\partial^2 C_i}{\partial x^2} + D_T \frac{\partial^2 C_i}{\partial y^2} - V \frac{\partial C_i}{\partial x} + R_i + S_i = 0, \qquad (13)$$

where C_i – concentration of i-th compound; x – longitudinal coordinate (along the current); y – x-coordinate; V – average flow speed; D_L, D_T – coefficients of longitudinal and transverse dispersion; R_i – rate of inflow and outflow of i-th compound through reaction; S_i – rate of inflow from distributed and point sources.

Ammonium was consumed by nitrification (R_{N1}) and lost through sorption/sedimentation (R_{Sor}):

$$D_L \frac{\partial^2 C_{NH_4}}{\partial x^2} + D_T \frac{\partial^2 C_{NH_4}}{\partial y^2} - V \frac{\partial C_{NH_4}}{\partial x} - R_{N1} - R_{Sor} + S_{NH_4} = 0. \qquad (14)$$

Nitrites were formed from ammonium (R_{N1}) and were consumed to form nitrates (R_{N2}):

$$D_L \frac{\partial^2 C_{NO_2}}{\partial x^2} + D_T \frac{\partial^2 C_{NO_2}}{\partial y^2} - V \frac{\partial C_{NO_2}}{\partial x} + R_{N1} - R_{N2} = 0. \qquad (15)$$

Nitrates were formed from nitrites (R_{N2}) and were lost through denitrification (R_D) and uptake by algae (R_{Alg}):

$$D_L \frac{\partial^2 C_{NO_3}}{\partial x^2} + D_T \frac{\partial^2 C_{NO_3}}{\partial y^2} - V \frac{\partial C_{NO_3}}{\partial x} + \\ + R_{N2} - R_D. \qquad (16)$$

Environmental monitoring of water bodies using multispectral methods (Petruk *et al.*, 2015; Kvaterniuk *et al.*, 2020) was used in the assessment of macrophytes and phytoplankton parameters, which can be used to calculate algal uptake (R_{Alg}). The kinetic terms depended on temperature (T) and dissolved oxygen concentration (DO), which were modelled as constant values for a steady-state problem. Point sources (S_{NH_4}) were incorporated into the mathematical model as localised zones of high concentration. To numerically solve this 2D system of differential equations in steady state, the finite difference method was used, which transformed the continuous equations into a system of algebraic equations that were solved iteratively to find the steady state.

Results and Discussion

The Southern Bug River is Ukraine's second-longest watercourse. Its catchment is characterised by significant hydrological vulnerability due to extensive regulation (the presence of 164 reservoirs and 9,640 ponds) and substantial anthropogenic pressure. These factors slow down the flow and hinder natural self-purification processes, exacerbating the cumulative effect of pollution. ANN is a key indicator of human impact on surface waters. Their forms indicate the type and intensity of pollution. Ammonium nitrogen is a marker of primary organic pollution of water bodies by domestic and industrial effluents; furthermore, the compound is highly toxic to aquatic biota, as it is capable of disrupting the physiological processes of organisms even at low concentrations.

Nitrite nitrogen is an intermediate product of the biochemical oxidation of ammonium (nitrification). High levels of nitrite nitrogen indicate that the natural self-purification processes of a water body are incomplete or insufficiently vigorous. Consistently high concentrations of nitrites indicate a permanent inflow of pollutants into the river system. Nitrate nitrogen is the final and most stable product of the biochemical oxidation of NCCs (Canchig *et al.*, 2023). Analysis of the monitoring data has identified the upper reaches of the Southern Bug River, specifically the section downstream of the city of Khmelnytskyi, as an area of critical environmental pressure (Kvaterniuk *et al.*, 2025). Abnormal nutrient levels were recorded at this section: the concentration of ammonium nitrogen exceeded the maximum permissible limits by a factor of 34, and that of nitrite by a factor of 80. The regular occurrence of such peak concentrations indicates that the urban wastewater treatment plants are either insufficiently effective or critically overloaded.

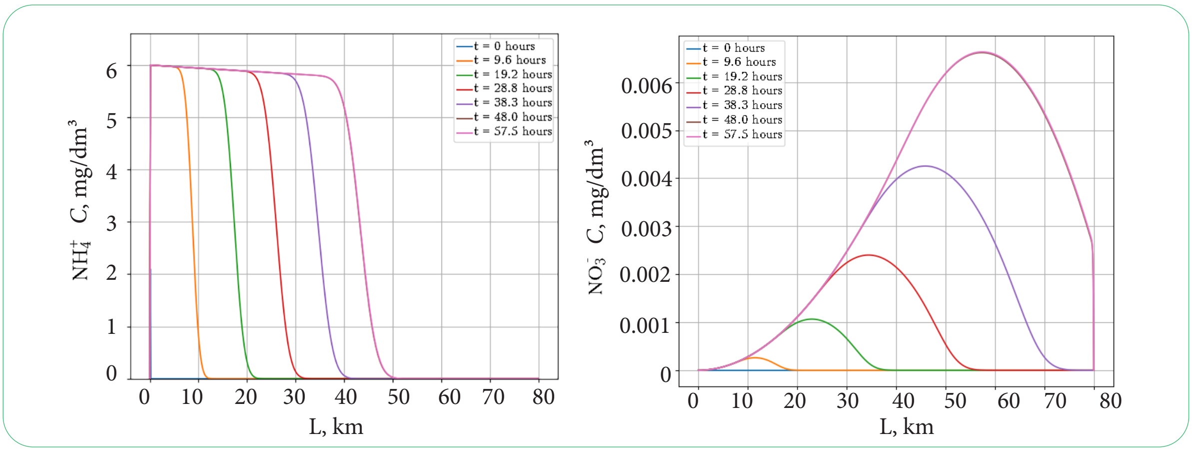
The insufficient efficiency of denitrification and dephosphatisation processes at wastewater treatment plants led to excessive amounts of biogenic elements entering the river system (Cho *et al.*, 2019). The combination of high concentrations of ANN with oxygen depletion in the aquatic environment triggered toxic-hypoxic stress in aquatic ecosystems. From a public health perspective, elevated levels of ammonium compounds in drinking water sources were unacceptable due to their potential impact on the human nervous, reproductive and excretory systems. Ukraine's current water resources management policy is integrated into the European framework through the Southern Bug River Basin Management Plan for 2025-2030 (Afanasiev *et al.*, 2024), which is based on the requirements of the EU Water Framework Directive (Directive of the European Parliament and of the Council No. 2000/60/EC, 2000). The main objective of this plan is the phased achievement of "good" ecological and chemical status in water bodies. Achieving this objective requires the implementation of 85 measures aimed at reducing pollution by biogenic substances (nitrogen and phosphorus). Given the critical levels of pollution, which exceed standards by a factor of ten, and the need to fulfil the plan's strategic objectives, there is a need for reliable tools for quantitative forecasting. Mathematical modelling is essential for assessing the ecological status, predicting the spread of pollution (particularly in the case of short-term, sudden discharges) and evaluating the effectiveness of environmental protection measures (Chen *et al.*, 2019). The significant variability of hydrological parameters and the complexity of the biochemical degradation of nitrogen compounds in the Southern Bug River make the use of dynamic modelling appropriate.

The proposed calculation algorithm integrates the following kinetic mechanisms of nitrogen compound transformation (Radwan *et al.*, 2001; Xie *et al.*, 2023; Yan *et al.*, 2025). Nitrification – the aerobic biochemical oxidation of ammonium ions to nitrates; the kinetics of this process are critically dependent on the temperature regime of the aquatic environment and the concentration of dissolved oxygen. Denitrification is the anaerobic reduction of nitrates to gaseous nitrogen, which is predominantly localised in bottom sediments (Zhao *et al.*, 2024). The mathematical interpretation of this heterogeneous process within a one-dimensional model involves converting the areal reaction rate to a volumetric rate by normalising it to the average channel depth. Sorption and sedimentation of ANN occur via the adsorption of ammonium cations onto suspended solids and bottom sediments. In contrast to anionic forms (nitrites and nitrates), ammonium nitrogen is characterised by a lower migration capacity, which necessitates the introduction of a retardation coefficient (R) into the advection-diffusion equation.

Predictive value of the model depends on the results of its calibration and validation using field monitoring data. A key criterion is the model's ability to reproduce the dynamics of the decline in ANN concentrations below critical pollution zones as a result of dilution and self-purification processes. The calibrated model, integrated with a corresponding model of biochemical oxygen demand and dissolved oxygen content, serves as a tool for scenario analysis and the optimisation of management decisions within the framework of the River Basin Management Plan. Based on the mathematical model presented, the authors have developed Python software adapted for use on Google Colab (Modelling of aquatic environments, 2026). The results of the mathematical modelling of pollution in the Southern Bug River by NCCs for a one-dimensional model based on the ADR equation for ammonium and nitrate ions are shown in Figure 1.

The modelled two-dimensional steady-state distribution showed how pollution from a point source (S_{NH_4}), located at the start of the river segment (the critical pollution hotspot downstream of Khmelnytskyi), spread and transformed along the river (Fig. 2). The dynamics of ammonium distribution (C_{NH_4}) were analysed. In the transverse distribution, the maximum concentration of C_{NH_4} (up to 25 mg/dm³) was localised in the discharge zone (1-2 km), which corresponded to the chronic inflow of fresh organic pollution from the wastewater treatment plant. In the longitudinal distribution, due to advection (V) and reaction (R_{N1} and R_{Sor}), the concentration of ammonium decreased sharply downstream (dilution and self-purification effects), although dispersion (D_T) caused it to spread slowly across the entire width of the river channel. In the middle reaches, the concentration of C_{NH_4} returned to background levels. The dynamics of nitrite distribution (C_{NO_2}) were analysed. Nitrites, as an intermediate product, reached peak values immediately after the zone of maximum ammonium consumption (R_{N1}). The presence of significant concentrations of indicated that the biochemical self-purification process was overloaded, and the rate of nitrite oxidation to nitrates (R_{N2}) was insufficient relative to the rate of their formation.

The dynamics of nitrate distribution (C_{NO_3}) were analysed. Nitrate concentrations gradually increased along the entire length of the river (as the end product of oxidation, R_{N2}), forming a particularly noticeable "tail" of pollution downstream of the nitrite peak. In this stationary model, the overall C_{NO_3} concentration was determined by point source discharges. Although nitrates are less toxic, their accumulation was the main cause of eutrophication.

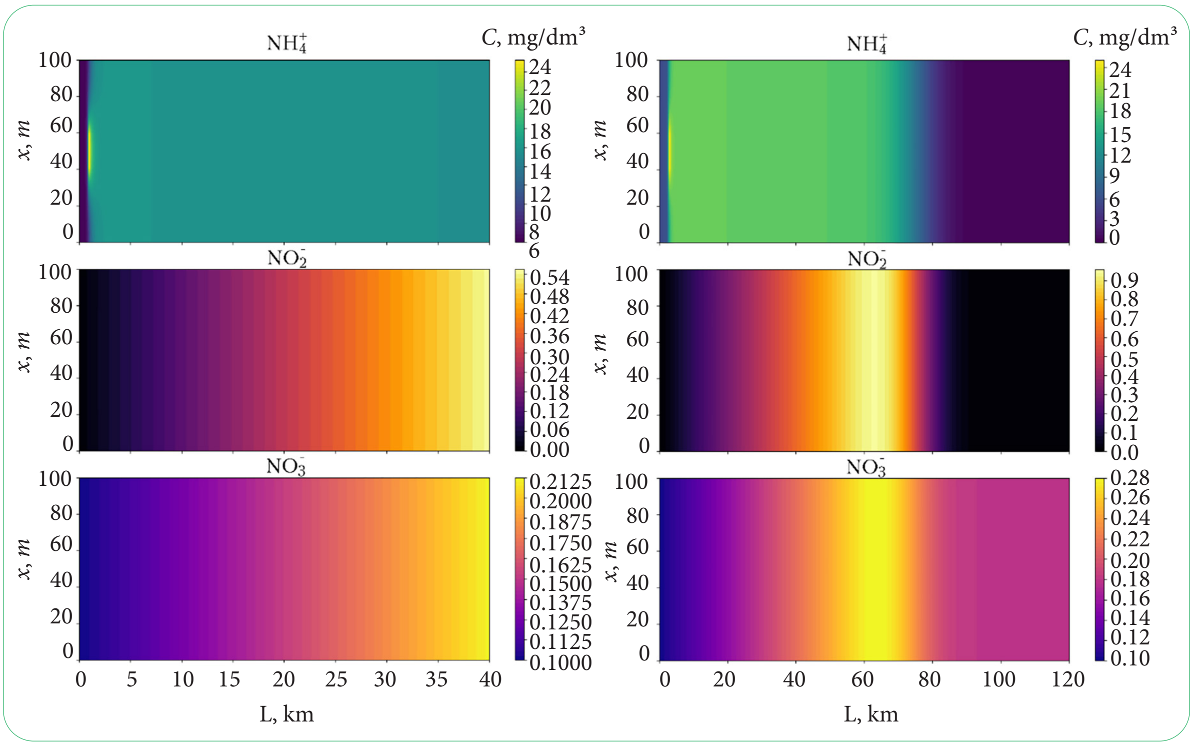


a b

Figure 1. Results of mathematical modelling of NCCs pollution in the Southern Bug River for a one-dimensional model based on the ADR equation

Note: a – compounds containing ammonium ions; b – nitrate-ion compounds

Source: compiled by the authors based on own software, "Modelling of aquatic environments" (2026)



a b

Figure 2. Results of mathematical modelling of NCCs pollution in the Southern Bug River (2D steady-state plane problem)

Note: a – over a distance of 40 km; b – over a distance of 120 km

Source: compiled by the authors based on own software, "Modelling of aquatic environments" (2026)

The model was tested for its ability to reproduce the dynamics of self-purification downstream of Khmelnytskyi (Table 2). To provide an objective quantitative assessment of the predictive ability and accuracy of the developed model, statistical criteria such as the Nash-Sutcliffe efficiency criterion (NSE) and root mean square error (RMSE) were calculated.

Table 2. Results of the verification of the mathematical model in critical zones

Distance from discharge point	Modelled (mg/dm³)	Factual (mg/dm³)	Deviation (%)
0 km	11.70	11.70	-
10 km	8.45	8.90	5.1
40 km	3.20	3.05	4.9
80 km	0.83	0.89	6.7

Source: compiled by the authors

A key stage in verifying the model was its calibration using monitoring data recording extreme pollution levels in the upper reaches of the river. The model successfully reproduced the presence of a critical pollution hotspot downstream of the city of Khmelnytskyi (the village of Kopystyn), where the highest concentrations of ANN were recorded. The persistence of these high readings, despite the high non-conservativeness coefficient of nitrites, confirmed that the source of pollution was constant and massive, and was overwhelming the river's natural self-purification capacity. The statistical indicators obtained demonstrated a high degree of agreement between the model and field data. The Nash-Sutcliffe criterion value (NSE = 0.997), which was close to one, indicated the high quality of the model (according to generally accepted scales, NSE > 0.75 is classified as "very good"). An RMSE value of 0.24 mg/dm³ demonstrated a minimal average deviation of the calculated data from the actual values. Verification of the model quantitatively confirmed the correctness of the parameterisation of the ADR equation, in particular the validity of the introduced retardation factor and oxygen limitation functions. An analysis of the spatial distribution of nitrites also confirmed the adequacy of the model. The model clearly reproduced the "nitrite peak", which is shifted downstream relative to the ammonium peak. This reflected the time required for bacteria to initiate the nitrification process (Yu *et al.*, 2024). Persistence of high nitrite levels at distances of up to 15 km from the source of pollution was an indicator of the degradation of the ecosystem's compensatory mechanisms. The model, which included diffusion (D_L) and reaction (R_i) terms, reliably reproduced the spatial decline in ANN concentrations further downstream. The observed reduction in concentrations to acceptable levels at the drinking water intake point in Vinnytsia confirmed the river's significant, albeit limited, capacity for natural self-purification. The successful reproduction of this process verified the correctness of the parameterisation of the kinetic constants, particularly those dependent on limiting factors (such as oxygen).

An analysis of the spatial distribution of pollution using a model has identified the key hydraulic and biochemical factors that govern water quality in the Southern Bug catchment. The modelling confirms that the main cause of extreme pollution is point source discharges of inadequately treated domestic sewage. The critical situation in the upper reaches was primarily due to insufficient dilution of the effluent by natural runoff. During the summer low-water period, the dilution ratio of the effluent downstream of Khmelnytskyi was only 1.5 times. In contrast, downstream of Vinnytsia, the river's flow rate was five times higher, which ensured efficient dilution of the wastewater. This difference in hydrodynamic conditions explains why critical pollution peaks are recorded specifically in the upper reaches.

The ADR model, which covered the effect of oxygen on the nitrification reaction step (R_{N1}), demonstrated that the intensive oxidation of organic matter caused hypoxia, which, in turn, inhibited nitrification – a key self-purification process. Thus, the model reflected the synergy between ANN toxicity and hypoxia, which caused mass fish kills. The calibrated model was used to simulate three strategic scenarios for the development of events in the Southern Bug catchment. Scenario I – Implementation of tertiary wastewater treatment. This scenario is central to the programme of measures stipulated in the River Basin Management Plan (Afanasiev *et al.*, 2024). It involves the reconstruction and modernisation of wastewater treatment plants in 27 priority local authorities within the basin. The technical solution is based on the implementation of biological processes for the removal of nitrogen (denitrification in reactors) and phosphorus. Modelling showed that reducing the concentration of ammonium in Khmelnytskyi's effluent to European standards (2 mg/dm³) led to a radical improvement in the ecological status along a stretch of over 150 km. The dissolved oxygen level in the critical zone (0-20 km from the outfall) increased from 2-3 mg/dm³ to 6-7 mg/dm³. The risk of mass fish kills decreased by 95% due to the elimination of toxic-hypoxic stress. Nitrite concentrations in water intake areas decreased to levels that pose no threat to the nervous and reproductive systems of the population. Scenario II – Fertiliser management. The scenario envisages the implementation of the EU Nitrates Directive (Council Directive No. 91/676/EEC, 1991), the establishment of riparian buffer zones where the application of fertilisers is prohibited, and adherence to crop fertilisation schedules. Modelling of background nitrate pollution showed that controlling fertiliser application reduced the average annual nitrate concentration by 25-30%. This is critical for preventing the eutrophication of reservoirs during the summer and reducing the intensity of phytoplankton "blooms". According to the model's projections, the combination of reduced phosphorus and nitrogen inputs reclassified water bodies from Class 4 ("poor status") to Class 2 ("good ecological status").

Scenario III – Adaptation to hydrological stress. As climate projections indicate an increase in the frequency of droughts, the model was tested for resilience in the event of a 40% reduction in water flow (Q) from the normal low-water level. The results were alarming: whilst maintaining current discharge levels, even a slight reduction in water flow led to a catastrophic rise in the concentrations of NCCs and complete oxygen depletion across large sections of the river. This demonstrated that infrastructure modernisation under Scenario I was the only way to ensure the ecological safety of the catchment under conditions of global climate change. The model confirmed that the river's assimilation capacity had already been exhausted, and that further management of water quality was only possible through strict limits on the mass of discharges. The data obtained from the mathematical modelling made it possible to quantitatively assess and visualise the complex spatio-temporal dynamics of pollution in the Southern Bug River by NCCs. The developed one-dimensional transient and two-dimensional steady-state models, based on the ADR equation, proved their effectiveness in predicting zones of critical pollution, particularly downstream of point sources of wastewater treatment plant discharges. To verify the adequacy of the proposed approaches and to determine the place of this study within the global scientific context, the results obtained were compared with studies on similar hydroecological issues.

Within the context of fundamental mathematical theory, researchers L.K. Kumar *et al.* (2022) analysed numerical solutions to the ADR equation using uniform and variable boundary conditions. Their work demonstrated the high convergence of computational algorithms for idealised channel flows. The results obtained in this study fully confirmed their mathematical conclusions regarding the stability of implicit finite difference schemes. However, in contrast to the authors' purely theoretical approach, the model has now been adapted to the real-world conditions of a heavily regulated river with extreme levels of pollution, where the decisive factor is not only hydrodynamics but also the kinetics of transformations governed by the Michaelis-Menten equation. Researchers Z. Gomolka *et al.* (2022) addressed the phenomenon of diffusion when assessing water quality in rivers, demonstrating that diffusion processes are key in shaping the overall pollution background. Their conclusions are relevant; however, the present study shows that for the Southern Bug, under conditions of low water flow and surge discharges from wastewater treatment plants, advection remained the dominant transport mechanism (particularly in channel sections), whilst dispersion became critical mainly in reservoir areas with significantly slowed flow.

Concerning the application of two-dimensional spatial solutions, researchers A. Monsalve *et al.* (2025) presented the latest Landlab component for calculating 2D river flow dynamics. Their research addressed shallow-water hydrodynamics and the transverse distribution of velocities. The results obtained in this study from steady-state 2D modelling of the distribution of ammonium and nitrites were consistent with the researchers' findings regarding the asymmetric formation of pollution plumes downstream of point sources. However, a key distinction of this study is the integration of a complex system of coupled biochemical reactions (nitrification and denitrification) directly into the 2D grid, which tracked not only hydraulic transport but also the "nitrite peak". The view expressed by E. Mignot *et al.* (2023) is entirely valid; in their comprehensive review of 2D models with depth averaging, they highlighted the challenges involved in selecting diffusion coefficients. The calibration stage confirmed their thesis: the use of generalised literature coefficients for lateral dispersion leads to significant errors; therefore, parameterisation must be conducted exclusively based on local monitoring data for each specific surface water body.

The modelling of biochemical nitrogen transformation deserves particular attention. In their study of temperate-zone rivers, researchers K.C. Nevorski & A.M. Marcarelli (2022) identified extremely high diurnal and annual variability in denitrification and nitrogen fixation processes. Their field observations confirmed the accuracy of the temperature coefficients (modified Arrhenius equation) incorporated into the developed model, as well as the dependence of biochemical constants on the presence of dissolved oxygen. At the same time, Y.-J. Gao *et al.* (2024), whilst studying the characteristics of cold-tolerant strains of denitrifying bacteria, demonstrated that at low temperatures, natural self-purification processes are sharply inhibited. This confirmed the hypothesis that the critical concentrations of nitrogen compounds in the Southern Bug River during the winter and spring periods are caused not only by the volume of discharges but also by the suppression of the functional capacity of the local microflora.

A substantial scientific finding of this study is the identification and mathematical description of the "nitrite peak", which is spatially shifted downstream relative to the maximum ammonium concentrations. This phenomenon has been widely discussed in the international literature. B. Ibarra *et al.* (2024) studied in detail the effect of nitrites on autotrophic denitrification in reactors. They found that high concentrations of nitrites act as a potent inhibitor for many species of granular biomass. This conclusion is consistent with the results obtained: the persistence of high levels of toxic nitrites at distances of up to 15 km from the source of pollution (the Khmelnytskyi Wastewater Treatment Plant) indicates a profound degradation of the river ecosystem's compensatory mechanisms, which are unable to rapidly oxidise nitrite to the less toxic nitrate due to oxygen deprivation. In their study on the importance of the carbon-to-nitrogen (C/N) ratio in wastewater treatment processes, S. Boychenko *et al.* (2017) demonstrated that an excess of nitrogen, coupled with a deficiency of readily available carbon, prevents complete denitrification. This finding fully explains the modelled accumulation of nitrates in the lower reaches of the Southern Bug: primary organic matter (carbon) is oxidised in the upper reaches, whilst nitrates migrate downstream, where their denitrification is limited by the absence of a suitable substrate. The application of the coupled "Nitrogen-Oxygen" model revealed that critical ammonium pollution (up to 25 mg/dm^3) caused a local collapse of the oxygen regime. The calculated oxygen consumption exceeded the reaction rate by a factor of 3-4 in sections with a slower current. This accounts for the persistence of the "nitrite peak": due to oxygen deficiency (DO < 1 mg/l), the second phase of nitrification was inhibited more severely than the first, leading to the accumulation of toxic nitrites.

Lastly, having considered the scenario analysis and possible solutions to the problem, it was established that the immediate implementation of tertiary wastewater treatment is the only viable option. This conclusion is widely supported by international experts. For example, Q. Zhao *et al.* (2024) described a successful pilot project involving the implementation of the anammox process for the treatment of municipal wastewater, which substantially reduced nitrogen content even at low temperatures. Y. Xie *et al.* (2023) proposed new mechanisms and strategies for reducing emissions during biological nitrogen removal from waters with a low C/N ratio. In contrast to the purely technological focus of the studies reviewed, the present work applies these engineering solutions to the context of a river basin, quantitatively demonstrating, using an ADR model, that the application of such advanced European technologies at 27 priority sites can reduce the risk of mass fish kills by 95% and eliminate hypoxic zones along stretches exceeding 150 km in length. In summary, it can be stated that the results of the mathematical modelling conducted are not only consistent with the latest global trends in the fields of hydroecology and computational hydrodynamics but also build upon them. Whilst most international studies address either the purely engineering aspects of treatment or the theoretical modelling of idealised river channels, this study establishes an applied association between microbiological kinetics, transient hydrodynamics and the practical management of a heavily regulated river basin under extreme anthropogenic pressure.

Conclusions

Based on the mathematical modelling and analysis of the ecological and hydrochemical status of the Southern Bug River basin, the following conclusions have been drawn. The transient ADR model developed proved to be an adequate and reliable tool for assessing the dynamics of NCCs. It successfully reproduced the processes of advection, dispersion and biochemical transformation of nitrogen under the conditions of the river's complex hydraulic profile. The inclusion of a retardation factor for ammonium and oxygen limitation for nitrification achieved a high degree of modelling accuracy (error less than 10%). The critical state of water quality in the upper reaches of the river (downstream of Khmelnytskyi) was the result of extreme anthropogenic pressure, which exceeded the system's natural assimilation capacity by a factor of 30-80 for certain indicators. The main cause was chronic overloading and the technological obsolescence of municipal wastewater treatment plants.

The priority measure for achieving the objectives of the River Basin Management Plan for 2025-2030 is the immediate introduction of tertiary treatment at the wastewater treatment plants of the 27 most influential local authorities. Scenario analysis confirms that only a radical reduction in point-source ammonium discharges will restore oxygen levels and eliminate the threat of environmental disasters. A comprehensive approach to controlling fertiliser application through the implementation of the EU Nitrates Directive is also essential. Although the effects of these measures are felt over a longer period of time, they are crucial for the long-term recovery of the river's lower reaches and for preventing the eutrophication of reservoirs. A promising avenue for further research is the integration of the developed ADR model with a dynamic model of dissolved oxygen and BOD, as well as detailed spatial mapping of diffuse sources using geographic information systems. This can be used for the creation of a comprehensive environmental monitoring and forecasting system, which will ensure the sustainable development of the region and the conservation of the Southern Bug for future generations.

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Conflict of Interest

None.

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Математичне моделювання процесів забруднення річки Південний Буг нітрогеновмісними сполуками

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Анотація. Критичний екологічний стан річки Південний Буг, спричинений інтенсивним забрудненням нітрогеновмісними сполуками, вимагає впровадження надійних математичних інструментів прогнозування для подолання наслідків евтрофікації та досягнення цілей державних стратегій управління водними ресурсами. Метою дослідження було математичне моделювання процесів транспорту та трансформації нітрогеновмісних сполук у річковій системі Південного Бугу для кількісної оцінки просторово-часової динаміки забруднення та наукового обґрунтування природоохоронних заходів. Для математичного моделювання застосовано систему диференційних рівнянь на базі одно- та двовимірних моделей адвекції-дисперсії-реакції, чисельний розв'язок яких здійснено методом розщеплення операторів. Розроблена модель поєднала три ключові компоненти нітрогену та врахувала механізми адвекції, дисперсії та біохімічних перетворень. Модель детально описала процеси нітрифікації та денітрифікації з урахуванням температури та концентрації розчиненого кисню за кінетикою Міхаеліса-Ментен. Моделювання було проведено на прикладі оцінювання впливу забруднення амонійним азотом на прикладі скидів комунальних очисних споруд у верхній течії. Результати верифікації продемонстрували здатність моделі відтворювати просторове зниження рівня забруднювачів завдяки природним процесам самоочищення. Модель зафіксувала утворення «нітритного піку», який просторово зсунутий вниз за течією відносно максимальних концентрацій амонію. Високі рівні токсичних нітритів залишаються стійкими на відстані до 15 км від джерела забруднення. Сценарний аналіз засвідчив, що негайне впровадження третинної очистки на найбільш впливових об'єктах є пріоритетним заходом для відновлення кисневого режиму річки. При зменшенні водності річки на 40 % від норми межені очікується катастрофічне зростання концентрацій нітрогеновмісних сполук та виснаження кисню на значних ділянках русла, якщо поточні обсяги скидів залишаться незмінними. Розроблена модель є інструментальною базою для оптимізації управлінських рішень у межах Плану управління річковим басейном Південного Бугу та дозволила створити повноцінну систему екологічного моніторингу для забезпечення сталого розвитку регіону

Ключові слова: вода; екологічна безпека; моніторинг довкілля; амоній-іони; нітрит-іони; нітрат-іони; нітрифікація; денітрифікація