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Entropy-weighted model for assessing the environmental safety of surface waters in the Southern Bug river basin

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ABSTRACT

Introduction. Ensuring the environmental safety of river basins is a critical challenge for Ukraine, particularly for strategically important waterways like the Southern Bug, which is subject to significant technogenic and agricultural pressure. Traditional assessment methods often rely on fixed weighting coefficients that fail to capture the local specifics of pollution. The aim of this study is to quantitatively assess the environmental safety of surface waters in the Southern Bug River basin using an entropy-weighted water quality index (EWQI), which accounts for the spatiotemporal variability and informational significance of hydrochemical indicators.

Methods. The study is based on a database of hydrochemical observations for the period 2020–2024, collected from 36 monitoring stations across the upper, middle, and lower reaches of the river. The analysis included 12 key water quality parameters. The methodology involved data normalization and the calculation of entropy weights using Shannon's information theory to determine the contribution of each parameter to the overall pollution level. Analytical tools included the calculation of seasonal EWQI values, spatial visualization using OpenStreetMap (OSM), Principal Component Analysis (PCA) for factor identification, and k-means clustering for zoning the basin.

Results. Spatial analysis revealed a distinct downstream gradient of water quality deterioration: from clean waters (Classes II–III, EWQI $\leq$ 1.0) in the upper basin to polluted and highly polluted waters (Classes V–VII, EWQI > 3.0) in the estuarine zone near Mykolaiv. A significant seasonal trend was established, with the mean EWQI increasing from 1.85 in the cold period to 2.46 in the warm period, indicating a 33% degradation in water quality due to intensified eutrophication processes. Entropy weight analysis identified ammonium (22%), phosphates (18%), and BOD_5 (15%) as the dominant contributors to the index, confirming the prevalence of biogenic and organic pollution. PCA results indicated that three factors – organic load, nutrient enrichment, and mineralization – explain more than 80% of the variance in the data.

Conclusions. The study confirmed that the entropy-weighted model provides an objective and sensitive tool for assessing aquatic ecosystems, effectively revealing spatial heterogeneity and seasonal risks. The research highlights that the warm season represents a period of critical ecological stress for the Southern Bug. The practical value of the model lies in its applicability for automated assessment and spatial mapping within the state environmental monitoring system, providing a scientific basis for optimizing monitoring networks and management decisions.

Keywords: *entropy-weighted index, environmental safety. water quality, Southern Bug River basin, hydrochemical parameters, seasonal dynamics, GIS, clustering, PCA, surface water monitoring.*

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Introduction

The problem of preservation and rational use of Ukraine's water resources remains one of the most pressing issues in the context of ensuring environmental safety, sustainable development, and adaptation to climate change. The condition of surface waters serves as an integral indicator of technogenic pressure on the environment, since water bodies accumulate pollution from industrial, agricultural, municipal, and transport sectors. Contemporary Ukrainian researchers emphasize that river basins act as the main receptors of anthropogenic discharges and secondary pollutants; therefore, their hydroecological state directly determines the level of regional environmental safety. The study [1] demonstrated that even under regulatory control of wastewater quality, environmental risks from domestic and industrial effluents remain significant, particularly due to the instability of treatment facilities and the overload of sewer systems in urban areas. Similar patterns are observed for the large basin systems of Ukraine, such as the Dnipro, Siverskyi Donets, and Southern Bug rivers. Within these catchments, there is an accumulation of biogenic compounds, organic substances, and heavy metals, which form persistent pollution zones and disrupt the biogeochemical balance [2, 3].

Research conducted during 2021–2023 revealed that the influence of technogenic sources on surface water quality has a systemic nature. In study [2], the concept of using composite indicators of water ecological safety was substantiated, integrating the cumulative effects of several groups of parameters: toxicological, biogenic, and organic. The developed approaches made it possible to quantify the degree of degradation of aquatic systems and to compare the ecological state of different basins. The authors emphasize that traditional index-based assessment methods (e.g., WQI) do not always reflect the real complexity of processes in aquatic environments, as they use fixed weighting coefficients insensitive to spatiotemporal variability.

Particular attention is paid to the Southern Bug River basin, one of the largest hydrological systems of Right-Bank Ukraine, which has crucial strategic, socio-economic, and ecological significance. The catchment area encompasses industrially developed regions with a high concentration of enterprises in machine-building, food, chemical, and energy industries, as well as vast agricultural lands. This land-use structure determines the combined nature of technogenic pressure-both point (from wastewater discharges) and diffuse (from agricultural runoff). The study [3] showed that such combined sources are responsible for the formation of complex multielement pollution systems, manifested in exceedances of the maximum allowable concentrations of ammonium nitrogen, phosphates, and organic substances, as well as in increased chemical oxygen demand (COD) and biochemical oxygen demand (BOD_5) values.

According to the integral assessment of the state of Ukraine's water bodies performed by the authors [4], the Southern Bug basin belongs to the category of environmentally stressed systems, especially during the summer–autumn period. During this time, a decrease in water flow, intensification of thermal stratification, and accumulation of pollutants in bottom layers are observed. Under low-water conditions and reduced water exchange, the highest values of the entropy-weighted integral pollution index are recorded, indicating ecosystem degradation and a reduction of its self-regulatory capacity.

The problem is aggravated by the fact that the existing system of environmental monitoring does not always ensure sufficient representativeness of the data. The frequency of sampling and the number of observation points are limited, while the interpretation of results often relies on expert judgments. Therefore, there is a need to develop formalized models capable of providing objective, quantitative, and automated assessment of the state of surface waters based on available hydrochemical parameters.

In this context, the application of the entropy-weighted approach appears particularly promising. It is based on Shannon's information theory and enables the determination of both the degree of system uncertainty and the informational significance of each water-quality parameter [2–4]. This method eliminates the subjectivity inherent in expert weighting, since the coefficients are calculated directly from empirical data, reflecting the internal structure of variations in hydrochemical parameters. The use of entropy-weighted indices allows not only the description of the current state of aquatic ecosystems but also the identification of degradation trends, zones of increased risk, and temporal phases of water-quality deterioration.

The scientific problem addressed in this study lies in the absence of regionally adapted models for assessing environmental safety in most Ukrainian river systems, including the Southern Bug. Existing approaches usually focus on nationwide generalizations, whereas this research proposes a localized assessment framework that accounts for the seasonal dynamics, spatial structure of the basin, and specific features of anthropogenic pressure. Unlike previous works, which emphasized aggregated assessments at the national scale, this study seeks to provide a detailed representation of processes within a single basin, considering its hydrological and anthropogenic particularities.

The development and testing of an entropy-weighted model for assessing the environmental safety of the Southern Bug River basin will make it possible to solve several applied tasks, namely:

- to ensure quantitative comparison of different river sections using a unified scale;
- to identify temporal phases of ecological stress;
- to enhance the substantiation of management decisions in the field of water-resource protection;
- to optimize the monitoring network by focusing resources on the most problematic areas.

The implementation of this approach is fully consistent with the objectives of the EU Water Framework Directive 2000/60/EC, aimed at achieving a "good ecological status" of water bodies, and it aligns with the United Nations Sustainable Development Goals (SDGs): SDG 6 "Clean Water and Sanitation", which calls for universal access to safe water and effective management of water resources; and SDG 12 "Responsible Consumption and Production", which focuses on reducing the environmental impacts of economic activities.

Thus, the study of the environmental safety of the Southern Bug River basin using the entropy-weighted approach has a dual significance: (1) scientific-methodological, as it expands the toolkit for quantitative evaluation of aquatic-system conditions; and (2) applied, as it provides the basis for improving water-resource management systems at the regional level and integrating the obtained results into national monitoring programs.

The assessment of the ecological state of water bodies is a complex task that requires comprehensive consideration of numerous factors: anthropogenic load, natural self-purification processes, seasonal variations in hydrological regimes, and the influence of climatic conditions. Over the past decade, the scientific community has focused on developing integrated indicators that enable the quantitative evaluation of the environmental safety of aquatic systems based on heterogeneous monitoring data [5].

In contemporary Ukrainian research, approaches based on assessing the ecological stability of catchment landscapes and bioindication are actively being developed alongside traditional hydrochemical methods. Specifically, the works of Malovanyy M. S. et al. have demonstrated a close correlational relationship between the coefficient of landscape ecological stability and the hydroecological status of river basins. Using the upper reaches of the Pripyat River basin as an example, the authors established that areas with a high proportion of stable landscape elements (forests, meadows) are characterized by higher Macrophyte Index (MIR) values and better water quality. Statistical analysis confirmed a strong inverse relationship ($r = -0.87$) between anthropogenic landscape pressure and integrated water quality indicators [6].

Studies of the biotic component conducted on the Siret and Turia rivers have shown the effectiveness of using the Macrophyte Index (MIR) and zooperiphyton indices (TBI, BMWP, saprobic index) for diagnosing the ecological status of transboundary rivers. It was found that different biotic indices might yield varied assessments for the same monitoring site (ranging from "polluted" to "very polluted" water), highlighting the necessity of employing integrated approaches [7, 8].

Concurrently, for the operative forecasting of technogenic loads, Ponomarenko R. V. et al. proposed the use of material balance mathematical models, which describe a linear dependence between the increase in pollutant mass and its concentration. It has been established that in actual water bodies, unlike in "pure dilution" conditions, self-purification processes or secondary pollution play a significant role, altering the nature of these dependencies for conservative and non-conservative substances. However, such deterministic models require extensive data sets, which are not always available under limited monitoring conditions [9].

Traditionally, to summarize large sets of hydrochemical parameters, researchers have applied index-based methods, the most well-known of which include the Water Quality Index (WQI), the Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI), and the National Sanitation Foundation WQI (NSFWQI). These approaches are widely used in both scientific and practical applications, as they allow the aggregation of monitoring results into a single integral indicator [10].

However, many scholars point out the limitations of classical indices. The weighting coefficients used in WQI formulations are typically defined through expert judgment, which reduces objectivity and makes the assessment dependent on subjective decisions. Moreover, such models are insufficiently sensitive to local dynamics–they do not adequately account for seasonality, variability, or interdependence among parameters [11].

The attempt to eliminate subjectivity in index construction has led to the development of methods based on the information-entropy approach. According to Shannon's theory, entropy represents a measure of uncertainty or disorder within a system. In the context of environmental monitoring, entropy characterizes the degree of informational variability of each parameter–that is, the extent to which a given indicator fluctuates in space and time. The higher the entropy, the lower its informational contribution to an overall evaluation, and vice versa.

In the study by Adimalla (2021), an entropy-weighted water-quality index was first applied to rivers in India, which enabled the elimination of subjective weights and increased the reliability of integral assessments [12]. Similar approaches have been implemented in Iran, China, India, and South Africa for the analysis of both surface and groundwater quality. In all cases, it was shown that entropy-weighted models reveal spatial variability and seasonal fluctuations of parameters more effectively than classical WQI models.

Specifically, Wang et al. (2021) demonstrated that when entropy-based weighting was applied, the coefficient of determination between computed indices and actual water-quality data increased from 0.72 to 0.89, confirming improved accuracy and stability of the method [13]. Thus, information-entropy approaches are now recognized as among the most effective tools for the assessment of complex natural-technogenic systems.

In Ukrainian scientific practice, the information-entropy approach has been actively developed over the past five years. Bezsonnyi, Plyatsuk, and co-authors proposed composite indicators of water ecological safety, in which parameter integration is carried out considering entropy-based weights calculated according to the variability of hydrochemical indicators [2]. These studies emphasize that entropy is a natural criterion for determining the significance of each parameter in the overall pollution structure, as it reflects the degree of its informational "saturation" and sensitivity to changes in the aquatic environment.

The development of information-entropy methods in water resources monitoring allows for overcoming the uncertainty inherent in traditional deterministic models. In the review paper by Bezzsonnyi V. L. (2023), the global experience of using Shannon's theory for designing monitoring networks is summarized, where entropy acts as a measure of the informational content of the data. It is demonstrated that the entropic approach facilitates the optimization of observation post locations and sampling frequency, based not on prescriptive regulations, but on the actual variability of hydrological and hydrochemical parameters [14].

A practical application of this approach was carried out for a drinking water supply source in the Dnipro agglomeration. The calculation of the Entropy-Weighted Quality Index (EWQI) revealed significant seasonal differentiation in water quality: index values deteriorated during the warm period due to eutrophication and secondary pollution processes, a phenomenon not always captured by traditional assessment methods [15]. This supports the thesis that the weights of parameters in integral indices should not be static but should reflect the degree of disorder (uncertainty) within the system during a specific season. It is precisely the consideration of the seasonal dynamics of entropic weights, substantiated in previous research, that forms the basis of the developed model for the Southern Buh River basin.

In paper [3], the authors presented the results of an integrated assessment of the sources of pollution of the Dnipro Reservoir, based on the combination of traditional indices and entropy-based weights. It was demonstrated that such models allow for a more objective identification of basins with the highest level of ecological risk. In subsequent works [4], the entropy-weighted approach was extended to all major river basins of Ukraine (Dnipro, Dniester, Danube, Southern Bug, Don, Vistula, and the rivers of the Black Sea and Azov Sea regions). The obtained results showed that the Southern Bug, as well as the Black Sea and Azov Sea basins, exhibited the highest values of the entropy-weighted integral pollution index (EWQI), while the Danube and Dnipro basins demonstrated relatively stable conditions.

Thus, within the framework of domestic studies, a methodological foundation for the quantitative entropy analysis of aquatic ecosystems has been formed, which enables the objective evaluation of water quality without the use of expert weighting coefficients and ensures better comparability of results across different regions.

Beyond monitoring studies, a crucial component in ensuring the ecological safety of river basins is the development of effective technologies to reduce pollutant input from both point and non-point (diffuse) sources. Specifically, the work of Havryshko M., Popovych O., and Malovanyy M. S. analyzed the impact of highly concentrated wastewater from the food industry on water bodies. The authors proposed combined biotechnological treatment schemes that allow for a significant reduction in the load of organic substances (BOD, COD) and nitrogen compounds, which, as shown in our research, are critical for the Southern Buh basin [16].

The problem of diffuse pollution, particularly runoff from urbanized territories and roadways, is addressed in the research by Ugnenko Ye. B. and Yurchenko V. O. The authors demonstrated the effectiveness of using natural zeolites for the sorption purification of surface runoff from oil products, a relevant approach for technologically burdened sections of river basins [17].

A deeper understanding of nitrogen transformation processes – a key element of eutrophication – is highlighted in the works of Yurchenko V. O. and Tsitlishvili K. O. These researchers substantiated the use of immobilized microbiocenoses in rotating biological contactor (RBC) systems for implementing nitrification, denitrification, and the anammox process. This allows for deep nitrogen removal even under conditions of high organic pollution concentrations, representing an important technological solution for improving the status of river ecosystems [18].

For managing water treatment and wastewater disposal processes, Shtepa V. M., Pliatsuk L. D., et al. proposed an ecological-energy criterion that enables the optimization of treatment plant operations by balancing the ecological safety of discharges with energy consumption. This approach correlates with the principles of sustainable development and the requirements of ISO 14001 standards [19].

Contemporary research increasingly underscores the critical necessity of accounting for military impacts when assessing the ecological safety of Ukrainian river basins. The destruction of hydraulic structures, such as the Kakhovka HPP, and the cessation of operations at the Dnipro HPP have led to significant alterations in the hydrological and hydrochemical regimes of the Dnipro River. As noted by Horoshkova L. et al. (2025), the elimination of the Kakhovka Reservoir initiated complex self-purification processes in the upper pools but simultaneously created risks of secondary pollution due to changes in flow velocity and oxygen regime [20].

Furthermore, military operations cause direct chemical contamination of water bodies. Bezzsonnyy V. and Nekos A. (2023) established that in active conflict zones (e.g., the Siverskyi Donets River basin), emergency discharges and infrastructure destruction lead to a sharp increase in organoleptic indicators and nitrogen-containing substances, posing carcinogenic and mutagenic risks to the population [21].

To monitor this specific type of pollution, including heavy metal contamination resulting from shelling and man-made accidents, innovative geophysical methods are proposed. Menshov O., Horoshkova L., et al. (2025) demonstrated the effectiveness of analyzing the magnetic susceptibility of bottom sediments and soils [22]. Their research in the Khortytsia National Reserve revealed abnormally high magnetic susceptibility values that correlate with the content of heavy metals (Zn, Cr, Cu, Ni), although in some cases, the lithogenic factor of the

Ukrainian Shield is dominant. This approach allows for the retrospective reconstruction of pollution history and the separation of natural and anthropogenic anomalies [23].

Beyond military factors, a potent anthropogenic driver of water quality degradation remains the fragmentation of river channels by artificial water bodies. Research by Hapich H. et al. (2022) on small rivers in the Dnipropetrovsk region (Zhovtenka, Nyzhnia Tersa, etc.) proved a close correlation (R2 = 0.62) between the coefficient of flow regulation and the level of mineralization [24]. The transformation of rivers into cascades of evaporating ponds leads to the transgression of mineralization standards by 7–12 times, necessitating a review of the feasibility of operating such hydraulic structures. Andrieiev V. et al. (2022) proposed simplified specific indicators for assessing management effectiveness, which confirmed that in the Steppe zone of Ukraine, ponds retain only 25% of the water volume while occupying 44% of the area, primarily acting as evaporators and concentrators of pollution [25].

The agricultural sector also exerts significant pressure on the ecological status of basins, particularly during wartime. Horoshkova L. et al. (2024) analyzed the war's impact on the agrarian potential of the Kherson region, noting that the destruction of irrigation systems and soil contamination necessitates the use of econometric models (such as the Cobb-Douglas function) to optimize fertilizer and pesticide loads, which directly influences diffuse runoff into river basins [26].

In recent international studies, there has been an increasing trend toward integrating entropy-based methods with GIS technologies, machine learning, and decision-making models. For instance, Zhang et al. (2020) proposed a combination of the entropy-weighted water-quality index and principal component analysis (PCA) for the Yangtze River Basin, allowing identification of the leading pollution factors and the creation of a spatially explicit model of index distribution [27]. Similarly, Bekele Emiru et al. (2025) developed an entropy-weighted index for surface waters in South Africa using Sentinel-2 satellite data, which made it possible to implement real-time spatial monitoring [28].

A comparative review of studies [29–32] indicates that in most cases, the entropy-weighted approach has proven highly effective in revealing the seasonal and spatial regularities of water-quality variation. This confirms the universality of the method for different types of aquatic ecosystems.

Despite significant progress in the theory and practice of entropy-weighted assessment, several unresolved issues remain. First, most studies are oriented toward national or global scales and do not adequately account for the specific features of individual river basins. Only a few works consider local hydrological conditions, notably those for the Dnipro Reservoir [3]. Second, domestic studies are mainly based on annual averages, which limits the ability to analyze seasonal dynamics. Third, there is a lack of integration with geographic information systems, which constrains the application of such models in practical water-resource management.

Therefore, the relevance of further research lies in developing a regionally adapted entropy-weighted model for assessing the environmental safety of the Southern Bug River basin, which would account for seasonal variability, spatial heterogeneity of hydrochemical parameters, and local sources of technogenic pressure. This scientific niche determines the purpose and novelty of the present study.

The aim of this research is to quantitatively assess the environmental safety of surface waters in the Southern Bug River basin using an entropy-weighted model (EWQI) that takes into account the spatio-temporal variability of hydrochemical indicators and their informational significance. This approach makes it possible not only to provide an integral characterization of water quality but also to identify the key factors determining the ecological state of the basin and its spatial heterogeneity.

To achieve this objective, the study addressed the following main tasks:

- to compile a database of hydrochemical observations of surface waters for the period 2020–2024 within the Southern Bug River basin, including a complete set of key water-quality indicators;
- to perform normalization of hydrochemical parameters and to calculate their entropy weights, reflecting the informational contribution of each parameter to the overall structure of system variability;
- to calculate the entropy-weighted water quality index (EWQI) for each monitoring station separately for the warm period (April–September) and the cold period (October–March);
- to construct interactive GIS-based maps of EWQI distribution using OpenStreetMap (OSM), determine water-quality classes (I–VII), and visualize seasonal and spatial differences across the basin;
- to conduct a comparative and correlation–statistical analysis of the obtained results, including the assessment of seasonal variability of EWQI, determination of individual parameters' contributions to the overall index formation, and verification of the statistical significance of differences between the warm and cold seasons;
- to perform additional analyses aimed at a deeper understanding of the spatial and factor-driven patterns of pollution, specifically: to construct a map of seasonal changes ΔEWQI (warm–cold period); to perform spatial clustering of monitoring sites by the

level of pollution; to evaluate seasonal entropy weights of indicators and compare them; to perform principal component analysis (PCA) in order to determine the dominant pollution factors;

- to synthesize the research results into an integrated assessment of the ecological state of the basin, identify critical sections with the lowest environmental safety levels, and justify priority directions for further monitoring and water-quality management.

Methods

The initial data for this research were derived from the official results of the State Monitoring of Surface Waters published by the State Water Resources Agency of Ukraine for the years 2020–2024. Within the Southern Bug River basin, data from 36 stationary observation posts were selected, covering the upper, middle, and lower reaches of the river. This spatial representativeness ensures the possibility of a comprehensive assessment of the surface-water condition throughout the basin.

The study considered twelve key hydrochemical indicators representing various types of aquatic pollution, namely: biochemical oxygen demand (BOD_5), chemical oxygen demand (COD), permanganate oxidizability, dissolved oxygen concentration, ammonium, nitrates, nitrites, phosphates, synthetic surfactants (SPAR), suspended solids, sulfates, and chlorides. These parameters are the principal indicators of anthropogenic load, organic pollution, biogenic processes, and overall mineralization of water.

To unify indicators expressed in different measurement units, the initial data were normalized in accordance with standard approaches used in entropy analysis. For most parameters, normalized values were calculated using the following formula:

$$y_{ij} = \frac{x_{ij} - x_{\min}}{x_{\max} - x_{\min}}, \quad (1)$$

where (x_{ij})represents the concentration value of the *i*-th indicator at the *j*-th monitoring site.

For the parameter “dissolved oxygen”, an inverse normalization was applied:

$$y_{ij} = \frac{x_{\max} - x_{ij}}{x_{\max} - x_{\min}}, \quad (2)$$

since a decrease in its concentration indicates a deterioration in the ecological condition of the water body.

After normalization, the data were divided into two seasonal subsets: the warm period (April–September) and the cold period (October–March). For each subset, the information entropy (E_j) of every parameter was calculated using Shannon’s formula:

$$E_j = -\frac{1}{\ln n} \sum_{i=1}^{n} p_{ij} \ln p_{ij}, \quad (3)$$

where (p_{ij}) is the relative share of the normalized parameter value in the sample.

Based on the calculated entropy values, weight coefficients (W_j) for each indicator were determined as follows:

$$W_j = \frac{1 - E_j}{\sum_{j=1}^{m} (1 - E_j)}. \quad (4)$$

The obtained weights demonstrated distinct seasonal differentiation: during the warm period, the influence of organic and biogenic pollution (ammonium, phosphates, BOD_5) prevailed, whereas in the cold period, mineralization processes (sulfates, chlorides, COD) played a more significant role.

The entropy-weighted water-quality index (EWQI) was calculated as an aggregated value combining the relative concentrations of parameters with their respective entropy weights. The computation followed the formula:

$$EWQI = \sum_{j=1}^{m} W_j \frac{I_j}{S_j}, \quad (5)$$

where (I_j) is the measured value of the *j*-th parameter, and (S_j) is its regulatory limit according to the Ukrainian standard DSTU 4808:2007.

The resulting indices characterize the integral level of pollution for each monitoring site and for each season. To facilitate comparison, mean seasonal values of EWQI were determined within every observation point.

For spatial interpretation, interactive maps of EWQI distribution were created using OpenStreetMap (OSM) and the Folium library in Python. Each monitoring site was marked with a color-coded symbol corresponding to a seven-class water-quality scale: I (EWQI ≤ 0.3) – blue; II (0.3–1.0) – green; III (1.0–1.5) – orange; IV (1.5–2.0) – pink; V (2.0–4.0) – red; VI (4.0–8.0) – dark red; VII (>8.0) – black.

In addition to the maps for the warm and cold periods, a ΔEWQI map (warm – cold) was generated to display the seasonal dynamics of pollution levels and to identify areas with the most contrasting changes in water quality.

To verify the statistical significance of seasonal differences, the nonparametric Mann–Whitney test was applied, confirming the reliability of differences between the warm and cold periods at the $p < 0.01$ level.

To identify spatial regularities in water quality, cluster analysis using the k-means method was conducted, which allowed the delineation of four main zones with similar EWQI profiles.

To reveal the structure of interrelationships among parameters, the principal component analysis (PCA) method was applied. The results showed that the main factors determining water-quality variability were: organic pollution (BOD_5, COD, dissolved oxygen); biogenic load (ammonium, phosphates, nitrates); mineralization processes (sulfates, chlorides).

The estimation of the relative contribution of individual parameters to EWQI formation indicated that the dominant influence belonged to ammonium (up to 22%), phosphates (18%), and BOD_5 (15%), consistent with the PCA results.

The reliability maps constructed from the model outputs made it possible to identify areas with unstable water-quality characteristics that require enhanced monitoring and adjusted sampling frequency in future studies.

Results

For each monitoring site within the Southern Bug River basin, the mean seasonal values of the entropy-weighted water quality index (EWQI) were calculated separately for the warm period (April–September) and the cold period (October–March). The obtained results showed that index values ranged from 0.4 (indicating clean water, Class II) to 6.8 (very polluted water, Classes VI–VII).

On average, for the entire basin, the mean EWQI value was 1.85 ± 0.12 during the cold period and 2.46 ± 0.18 during the warm period, indicating a 33% deterioration in water quality in summer compared to winter. This dynamic is attributed to the intensification of biogenic processes, reduced aeration, and higher water temperatures, which stimulate eutrophication processes.

Comparison of these values demonstrates a clear downstream gradient of increasing EWQI–from 0.4–0.6 in the upper reaches to >6.0 near the estuary–reflecting the cumulative impact of anthropogenic load along the river course. Conversely, in areas with predominantly natural flow regimes (upper reaches, tributaries near Haivoron–Ladyzhyn), consistently low index values were observed, corresponding to Classes II–III (clean or moderately polluted waters).

Table 1

Presents a fragment of the calculated mean seasonal EWQI values for selected monitoring sites within the basin

Monitoring station name	Coordinates (lat., lon.)	EWQI (cold)	Class	EWQI (warm)	Class	ΔEWQI	Interpretation
Ladyzhyn (upstream)	48.69, 29.24	1.12	III	1.78	IV	+0.66	Deterioration of water quality due to municipal wastewater impact
Pervomaisk (downstream)	48.04, 30.84	1.65	IV	2.45	V	+0.80	Zone of biogenic pollution
Voznesensk	47.56, 31.32	2.08	V	3.12	V–VI	+1.04	Eutrophication and low dissolved oxygen
Mykolaiv (estuary section)	46.97, 31.97	2.86	V	6.80	VII	+3.94	Extremely polluted area
Haivoron (upper reach)	48.33, 29.85	0.43	II	0.62	II–III	+0.19	Relatively clean water
Yuzhnoukrainsk (reservoir)	47.83, 31.18	0.78	II–III	1.25	III–IV	+0.47	Moderate increase in organic load

Note: ΔEWQI = EWQI (warm) – EWQI (cold)

Figure 1 illustrates the seasonal distribution of mean EWQI values across the Southern Bug River basin. As can be seen, during the warm period most monitoring points shift upward by one quality class (from "moderately polluted" to "polluted"), confirming the overall trend of seasonal deterioration in water quality.

The analysis of the obtained results confirmed that the seasonal variability of the EWQI index is statistically significant ($p < 0.01$, Mann–Whitney U test). This indicates that water-quality formation processes in the basin have a distinct seasonal component.

During the warm period (mean EWQI = 2.46), the main determinants are the increased inflow of biogenic compounds (ammonium, phosphates, nitrates) through surface runoff and the decrease in dissolved-oxygen concentration, which reduces the self-purification capacity of water. In the cold period (mean EWQI = 1.85), a relative improvement in water quality is observed, caused by reduced biochemical activity, seasonal dilution of wastewater, and weaker thermal stratification.

The mean increment ΔEWQI = +0.61 for most sampling points indicates that the warm season is characterized by a higher level of ecological risk. The most problematic zones remain the Mykolaiv and Voznesensk sections, where EWQI in the warm season reaches 5–7, corresponding to very polluted and extremely polluted waters (Classes VI–VII).

The calculated values of the entropy-weighted water-quality index (EWQI) were integrated into a geoinformation environment for spatial analysis.

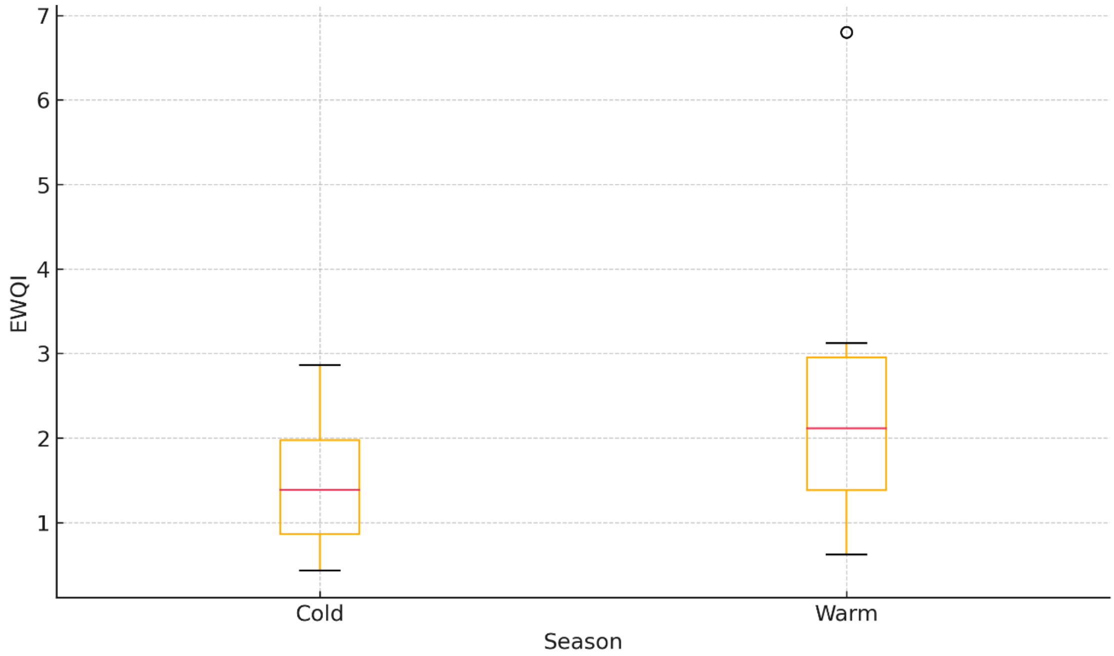

Fig. 1. Seasonal distribution of the entropy-weighted water-quality index (EWQI) across the Southern Bug River basin

Based on the coordinates of monitoring stations, two interactive maps (for the warm and cold periods) were created on the OpenStreetMap (OSM) platform, together with a ΔEWQI map showing the difference between warm and cold seasons.

The map for the warm period reveals a pronounced increase of EWQI in the middle and lower parts of the basin. Index values exceed 2.0 (Classes IV–V) in the areas near the cities Pervomaisk, Voznesensk, and Mykolaiv, indicating intensive organic and biogenic pollution. Meanwhile, the upper basin, particularly the Haivoron and Ladyzhyn regions, shows low index values (EWQI < 1), corresponding to Classes II–III–clean or moderately polluted waters.

On the cold-period map (Figure 3), the EWQI level decreases by approximately 0.3–1.0 units at almost all monitoring sites. The spatial structure becomes more uniform, and the proportion of areas classified as Classes IV–V is reduced by nearly half. This pattern indicates a seasonal self-purification of the river system, driven by reduced biochemical activity, lower surface runoff from agricultural lands, and the stabilization of the oxygen regime.

The map of seasonal changes in ΔEWQI (Figure 4) shows that the most intense deterioration in water quality (ΔEWQI > +1.0) occurs in the middle reach of the river–between Pervomaisk and Voznesensk–as well as in the estuarine zone near Mykolaiv. These areas can be considered critical zones of technogenic–ecological hazard, where the cumulative effects of industrial and agricultural discharges are most pronounced.

To identify spatial patterns and to group the monitoring sites by their ecological state, the k-means clustering method was applied to the dataset of EWQI values. The optimal number of clusters was determined using the Elbow criterion, which indicated the presence of four groups of water bodies with similar water-quality profiles (Table 2).

The analysis revealed that approximately 60% of monitoring sites belong to Classes III–V, indicating moderate to high pollution levels. At the same time, 17% of stations represent critical zones where EWQI exceeds 3.0, corresponding to very poor water quality. Mapping of cluster results allowed the delineation of five functional zones within the basin: Upper reaches – clean waters, low anthropogenic impact; Middle reaches – biogenic pollution from agricultural runoff and municipal sources; Tributaries – relatively stable zones with moderate quality; Urban–industrial areas – technogenically loaded, with high organic and nutrient inputs; Estuarine section – maximum ecological risk and cumulative pollution effects.

To identify the principal factors determining EWQI variability, a principal component analysis (PCA) was conducted. The first three principal components explained 82% of the total variance (Table 3).

The first factor (F1) reflects organic load associated with oxidative processes and shows the highest loadings for BOD_5, COD, and dissolved oxygen. The second factor (F2) represents nutrient (biogenic) pollution, primarily determined by ammonium, phosphates, and nitrates. The third factor (F3) characterizes mineralization processes, influenced by natural and anthropogenic inputs of sulfates and chlorides.

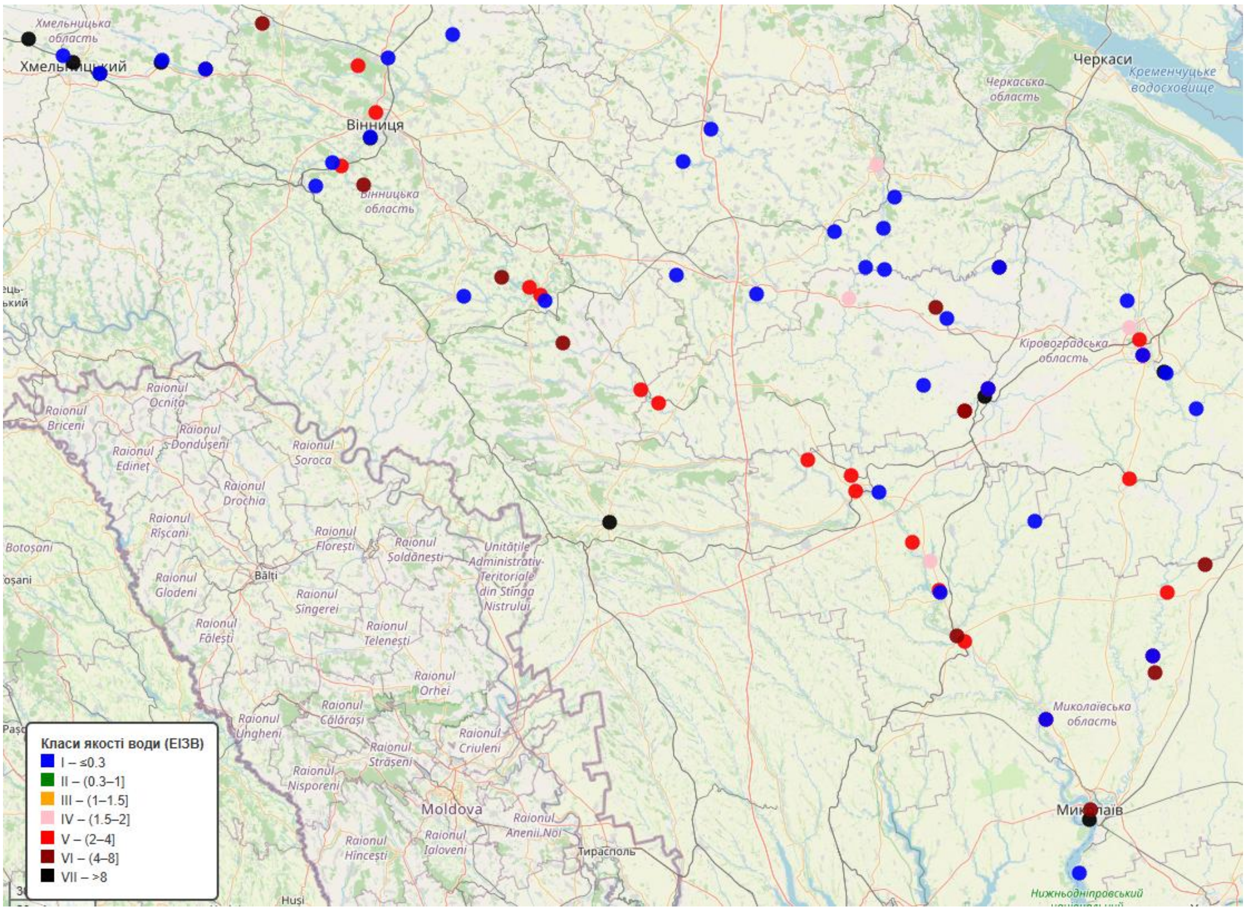

Fig. 2. Spatial distribution of the Entropy-Weighted Water Quality Index (EWQI) during the warm period (April–September) in the Southern Bug River basin

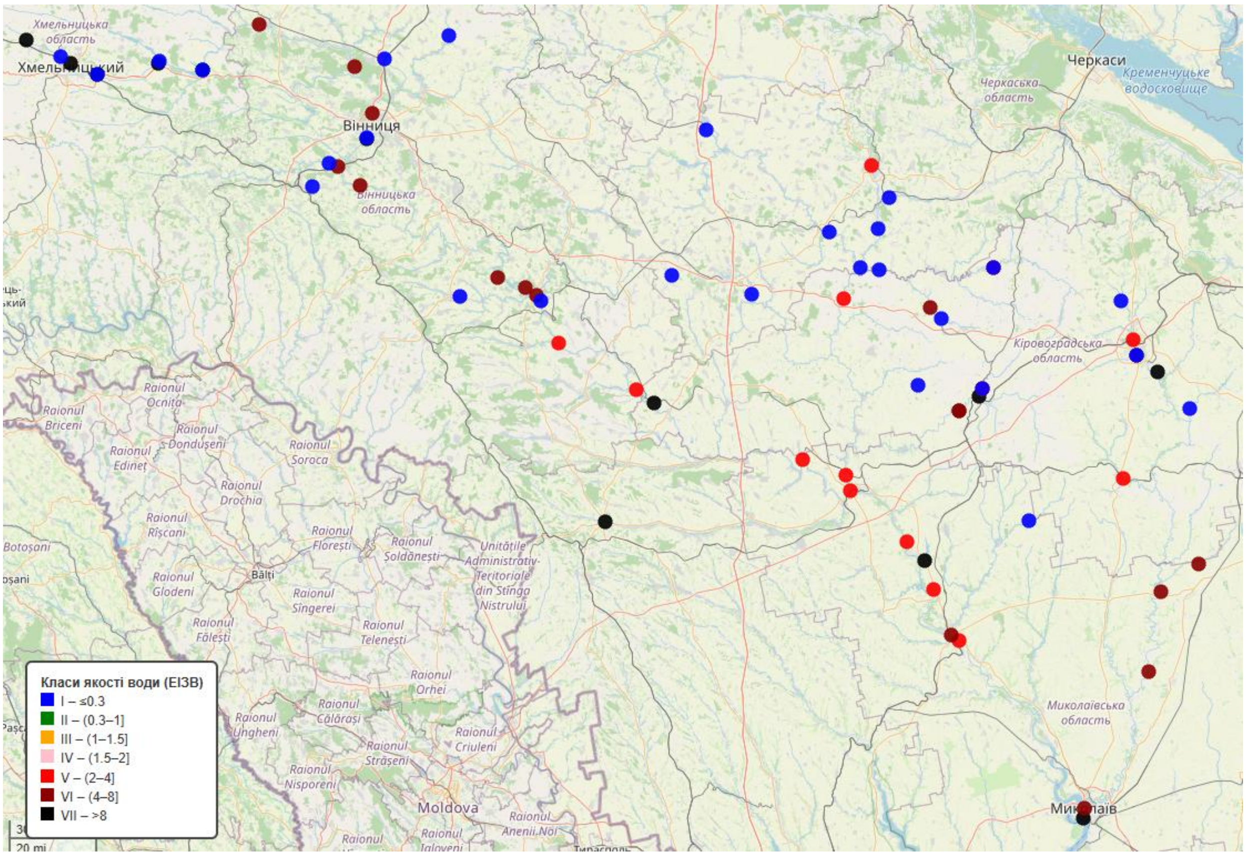

Fig. 3. Spatial distribution of the Entropy-Weighted Water Quality Index (EWQI) during the cold period (October–March) in the Southern Bug River basin

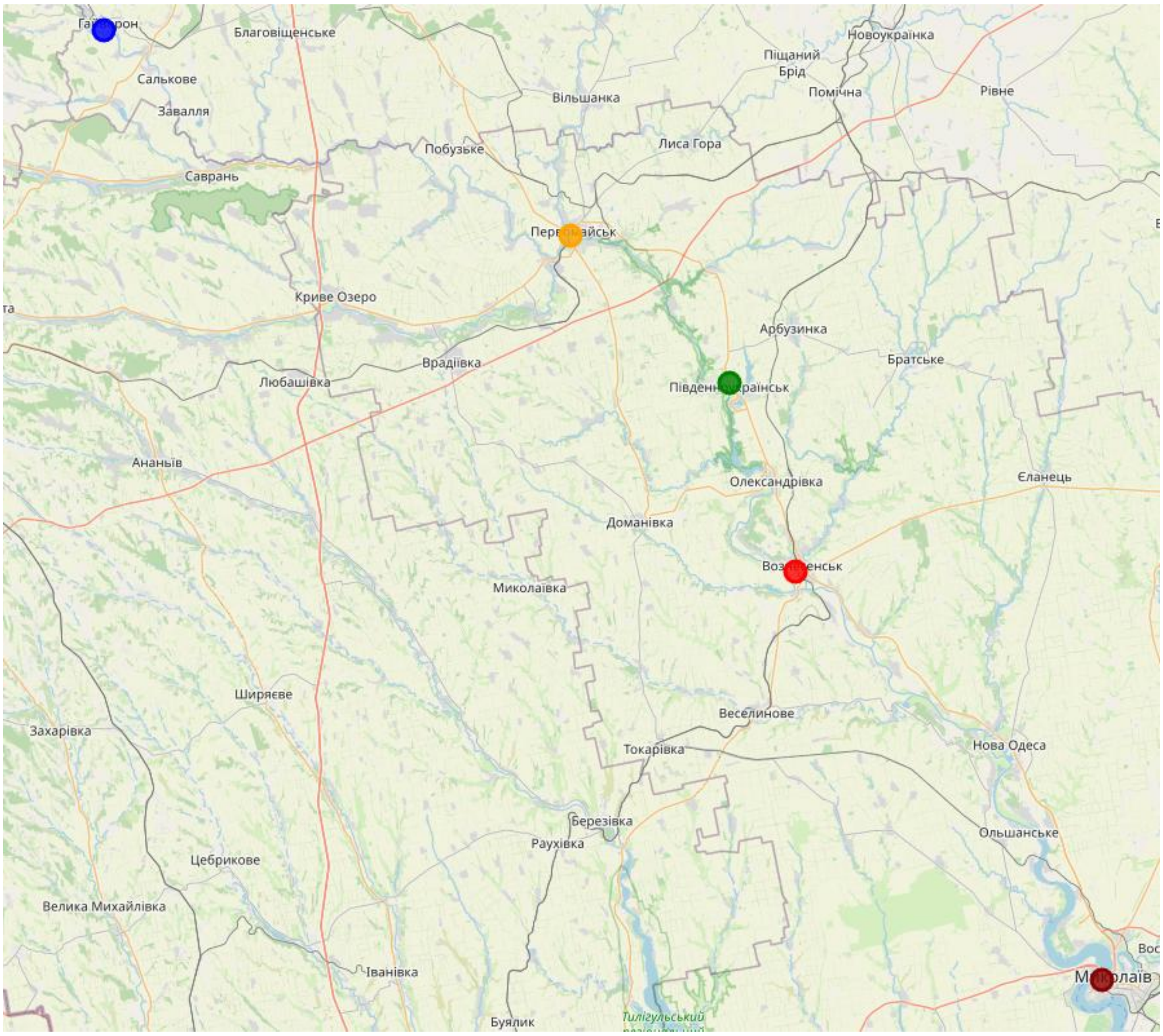

Fig. 4. Map of seasonal variations in the Entropy-Weighted Water Quality Index (ΔEWQI = EWQIwarm – EWQIcold) in the Southern Bug River basin

Table 2

Classification of monitoring sites based on the results of cluster analysis

Cluster	EWQI range	Water-quality characteristics	Typical sites	Share of sites, %
1	< 1.0	Clean or slightly polluted waters (Classes I–II)	Haivoron, Ladyzhyn	27
2	1.0–1.5	Moderately polluted (Class III)	Yuzhnoukrainsk, Trostianets	31
3	1.5–3.0	Polluted waters (Classes IV–V)	Pervomaisk, Voznesensk	25
4	> 3.0	Very and extremely polluted waters (Classes VI–VII)	Mykolaiv, estuarine section	17

Table 3

Factor loadings of principal components for hydrochemical indicators

Indicator	F1 – Organic load	F2 – Nutrient enrichment	F3 – Mineralization
BOD_5	0.89	0.21	0.12
COD	0.83	0.19	0.23
Dissolved oxygen	-0.77	-0.31	-0.18
Ammonium (NH_4^+)	0.34	0.87	0.09
Phosphates (PO_4^{3-})	0.27	0.81	0.15
Nitrates (NO_3^-)	0.22	0.76	0.29
Sulfates (SO_4^{2-})	0.11	0.18	0.84
Chlorides (Cl^-)	0.16	0.21	0.79

The resulting factor structure confirms that the environmental safety of the Southern Bug basin is primarily governed by a combined organic–biogenic pollution type. Seasonal analysis revealed that during the warm period, the importance of F2 (nutrient processes) increases, whereas in the cold period, F3 (mineralization) dominates–consistent with the natural hydrological and biochemical dynamics of the river system.

Based on the entropy weights and PCA results, the contribution of each indicator to the formation of the integral EWQI index was evaluated (Table 4).

Table 4

Contribution of main parameters to the formation of the entropy-weighted water-quality index (EWQI)

Indicator	Average entropy weight (W_i)	Contribution to EWQI, %	Type of impact
Ammonium (NH_4^+)	0.213	22.1	Biogenic pollution
Phosphates (PO_4^{3-})	0.172	17.8	Eutrophication effect
BOD_5	0.147	15.4	Organic load
COD	0.115	11.2	Chemical oxidation
Nitrates (NO_3^-)	0.096	9.1	Biogenic pollution
Dissolved oxygen	0.078	7.4	Inverse indicator of condition
Sulfates (SO_4^{2-})	0.072	6.9	Mineralization
Chlorides (Cl^-)	0.054	5.1	Salinity impact

The distribution of indicator contributions confirms that ammonium (22%), phosphates (18%), and BOD_5 (15%) are the dominant variables shaping the entropy-weighted index, aligning with the results of the PCA and the observed spatial patterns of biogenic and organic pollution across the basin.

Discussion

The combined contribution of the three key parameters (NH_4^+, PO_4^{3-}, and BOD_5) exceeds 55 %, indicating the decisive role of biogenic and organic pollution in shaping the environmental safety of the Southern Bug River basin. The spatial–seasonal and factor analysis demonstrated that the basin exhibits a mixed pollution pattern dominated by organic and nutrient compounds, especially during the warm season. The observed spatial heterogeneity is determined by the structure of land use: the upper reaches are mostly natural areas with low anthropogenic pressure, while the middle and lower reaches experience a persistent technogenic impact.

Both clustering and PCA confirmed that the water-use system and wastewater discharges are the principal factors degrading environmental safety. The obtained results have practical significance–they can be used to optimize the monitoring network, identify priority sampling sites, and develop targeted programs to reduce the biogenic load within the Southern Bug basin.

The results of the study confirmed that the entropy-weighted approach (EWQI) is an effective tool for quantitative assessment of the environmental safety of surface waters and for spatio-temporal analysis of the state of aquatic ecosystems. The proposed model not only provides an integrated evaluation of pollution levels, but also reveals the internal structure of processes determining water-quality variability across the basin.

The obtained EWQI values indicate a pronounced spatial heterogeneity and seasonal dynamics of hydrochemical conditions. The upper basin is characterized by stable water-quality parameters (Classes II–III), whereas the middle and lower reaches show a distinct increase in the index to Classes V–VII, reflecting substantial anthropogenic pressure.

The highest EWQI values were recorded in the Mykolaiv, Voznesensk, and Pervomaisk sections, whe-re during the warm period the index exceeds 6.0–classified as very polluted or extremely polluted waters.

Seasonal analysis revealed a consistent EWQI increase of 0.6–1.2 units in most sites during the warm period. This confirms the intensification of biogenic processes, the growth of ammonium, phosphate, and organic compound concentrations, and the resulting development of eutrophication phenomena. Conversely, during the cold period, the system shows relative stabilization of hydrochemical conditions, a reduction in nutrient load, and partial self-purification of surface waters.

The PCA results showed that over 80 % of total variance in the dataset is explained by three main factors–organic load, nutrient enrichment, and mineralization. This indicates that the ecological state of the basin is determined primarily by organic and biogenic pollution processes, intensified by anthropogenic activities such as industrial effluents, municipal wastewater, and agricultural runoff. At the same time, the mineralization factor dominates in the cold season, associated with the natural hydrogeochemical regime and low water exchange during winter.

Clustering of monitoring sites by EWQI made it possible to distinguish four ecological-state types that correlate with technogenic pressure and hydrological features. This approach enables optimization of the hydrochemical-monitoring network: in stable areas the number of stations may be reduced, while in zones of high variability (Classes VI–VII) it is advisable to increase the observation frequency and broaden the range of controlled parameters.

The practical value of the developed model lies in its potential integration into the environmental-safety management system of the basin at both regional and national levels. The derived EWQI indices can serve as: indicators of ecological risk reflecting the current state of surface waters; criteria for ranking river-network sections by pollution level; an information basis for constructing ecological-hazard maps, basin zoning, and defining priority monitoring directions; a core element of water-resource management systems, integrated with spatial databases and GIS platforms (e.g., QGIS, ArcGIS, Python GIS).

The developed approach also possesses predictive potential: combining entropy-weighted methods with machine-learning and time-series analysis could enable forecasting of water-quality changes under various water-use and climate-change scenarios.

Thus, the entropy-weighted model for assessing environmental safety is a universal and scientifically grounded instrument that enables objective evaluation, monitoring, and management of surface-water conditions.

Its implementation in the national environmental-monitoring practice will enhance decision-making efficiency, reduce the risk of aquatic-ecosystem degradation, and strengthen the environmental safety of the Southern Bug River basin as an essential component of Ukraine's national water policy.

Conclusions

An entropy-weighted model for assessing the environmental safety of surface waters (EWQI) was developed and tested using the case of the Southern Bug River basin. The model integrates Shannon's information entropy theory with normalized hydrochemical parameters, enabling an objective evaluation of water pollution levels while accounting for spatial and seasonal variability.

Based on calculations for 36 monitoring stations (2020–2024), mean EWQI values ranged from 0.4 (clean waters) to 6.8 (extremely polluted sections). The poorest water quality was observed in the middle and lower reaches of the river, particularly near Mykolaiv, Voznesensk, and Pervomaisk, where pollution levels corresponded to Classes V–VII.

Seasonal analysis revealed that during the warm period (April–September), the level of pollution increased on average by 0.6–1.2 EWQI units, caused by the intensification of biogenic processes, eutrophication, and a decline in dissolved oxygen concentration.

The entropy-weight analysis of weighting coefficients showed that the primary contributors to the integral index are ammonium (22%), phosphates (18%), and biochemical oxygen demand (BOD_5, 15%), indicating the dominance of organic and biogenic pollution types in the basin.

Principal component analysis (PCA) identified three key process groups determining the ecological state of the river: F1 – Organic load (BOD_5, COD, dissolved oxygen), F2 – Nutrient enrichment (NH_4^+, NO_3^-, PO_4^{3-}), F3 – Mineralization (Cl^-, SO_4^{2-}).

Together, these factors explain over 80% of the total variance in hydrochemical data.

Cluster analysis of water bodies revealed five functional zones of the basin: Headwaters – clean waters (Classes I–II); Middle reach – biogenic pollution (Classes III–IV); Tributaries – hydrochemically stable sections; Urbanized areas – technogenic pressure (Classes V–VI); Estuarine zone – areas of highest ecological risk (Classes VI–VII).

This spatial zonation forms a scientific basis for targeted water-quality management.

The interactive EWQI and ΔEWQI maps, created using OpenStreetMap (OSM), provide visual representation of seasonal and spatial pollution structures and can be used to support environmental decision-making.

The practical value of the proposed model lies in its potential integration into the national environmental monitoring system as a tool for operational control, risk assessment, and environmental planning within surface-water basins of Ukraine.

The scientific novelty of this study lies in combining the entropy-based approach with spatio-seasonal modeling and cluster–factor analysis, which improves both the accuracy and objectivity of ecological-safety assessments for aquatic ecosystems.

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Ентропійно-зважена модель оцінювання екологічної безпеки поверхневих вод басейну річки Південний Буг

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Метою дослідження є кількісне оцінювання екологічної безпеки поверхневих вод басейну річки Південний Буг на основі ентропійно-зваженої моделі (EWQI), що враховує просторово-часову мінливість гідрохімічних показників та їх інформаційну значущість. Було сформовано базу даних спостережень за 2020–2024 роки для 36 постів моніторингу та проведено нормування 12 основних показників якості води відповідно до ДСТУ 4808:2007. Ентропійні ваги розраховано за формулами Шеннона для визначення інформаційного внеску кожного параметра у загальний рівень забруднення. У результаті побудовано інтерактивні карти EWQI на основі OpenStreetMap для теплого (квітень–вересень) і холодного (жовтень–березень) періодів, а також карту сезонних змін ΔEWQI. Просторовий аналіз показав чіткий градієнт погіршення якості води вниз за течією – від чистих (класи II–III, EWQI ≤ 1,0) у верхів'ях до забруднених і дуже брудних (класи V–VII, EWQI > 3,0) у пригирловій частині. Середній рівень EWQI зріс із 1,85 у холодний період до 2,46 у теплий, що вказує на сезонне погіршення якості води на 33 %. Найбільший внесок у підвищення індексу мають амоній (22 %), фосфати (18 %) та $БСК_5$ (15 %), що відображає домінування біогенного й органічного забруднення. Аналіз головних компонент (PCA) показав, що три фактори – органічне навантаження, біогенне збагачення та мінералізація – пояснюють понад 80 % дисперсії даних. Просторова кластеризація дозволила виділити чотири типи екологічного стану річкових ділянок і зони критичного ризику в межах Миколаївської та Вознесенської ділянок. Основними обмеженнями дослідження є нерівномірна сезонна вибірка та обмежена кількість показників токсикологічного класу. Однак запропонована методологія може бути розширена шляхом інтеграції з геоінформаційними системами, машинним навчанням і супутниковими даними. Практична цінність моделі полягає у її придатності для автоматизованого оцінювання, картографування та управління якістю води у межах державної системи екологічного моніторингу. Наукова новизна полягає у поєднанні ентропійно-зваженого підходу, просторово-сезонного аналізу та факторної інтерпретації гідрохімічних процесів, що дозволяє підвищити об'єктивність оцінки екологічної безпеки водних екосистем.

***Ключові слова**: ентропійно-зважений індекс, екологічна безпека, якість води, басейн Південного Бугу, гідрохімічні показники, сезонна динаміка, GIS, кластеризація, PCA, моніторинг поверхневих вод.*

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