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Factor-cluster profiling of water quality in the Southern Bug Basin

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ABSTRACT

Introduction. The Southern Bug River Basin is one of the largest water-management systems of Right-Bank Ukraine, where natural runoff seasonality combines with sustained pressure from urbanized areas, agriculture, municipal wastewater, and industry. Existing studies either assess isolated water-quality indices, apply multivariate statistics without regulatory interpretation, or treat Ukraine at a generalized inter-basin level, so a reproducible basin-scale profile combining multiyear averages, seasonality, regulatory exceedances, and site typology is lacking for the Southern Bug. The purpose of the study was to perform factor-cluster and regulatory-index profiling of long-term hydrochemical series for rivers of the Southern Bug Basin, identifying reaches dominated by organic, nutrient, or mineralization-salinity pollution and ranking sites by hydrochemical risk. The object is surface waters of rivers within the Southern Bug Basin; the subject is the long-term structure of hydrochemical indicators, their seasonal variability, regulatory exceedances, and cluster profiles of monitoring sites.

Methods. The analysis used processed data of the state surface-water monitoring system of the State Water Agency of Ukraine for 13 January 2003 – 18 March 2026 (5,654 records, 95 sites). After plausibility control, 57 technical extremes were removed. Multiyear mean concentrations and seasonal profiles were calculated for organic-oxygen, nutrient, and mineralization-salinity blocks. Exceedance ratios and violation frequencies were computed against domestic-use and fishery-use reference values, and a screening index I₆ was built as the mean of the six highest partial exceedance ratios per site. Indicators were robustly standardized, visualized by principal component analysis, and grouped by k-means clustering.

Results. Under domestic-use reference values, the most frequent exceedances were COD (42.9% of samples), permanganate oxidizability (40.8%), and BOD₅ (14.8%). Under fishery-use reference values, violations were far more widespread: BOD₅ – 60.4%, COD – 42.9%, sulphates – 42.4%, permanganate oxidizability – 40.8%, nitrites – 31.5%, ammonium nitrogen – 18.8%. Seasonal profiles revealed oxygen-regime stress in summer (mean dissolved oxygen 7.60 mg/dm³ versus 10.80 mg/dm³ in winter), with higher COD and permanganate oxidizability in the warm period. PCA showed the leading components reflect nutrient enrichment and mineralization-salinity processes. Clustering of 48 sites yielded three profiles: organic-oxygen (43 sites, basin-wide background pressure),

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mineralization-salinity (3 sites), and nutrient (2 sites, upper reaches). The highest I6 values occurred near the Bug Estuary, the lower Inhul River in Mykolaiv, and the upper Southern Bug downstream of Khmelnytskyi; under fishery-use values, upper-basin sites showed a sharp risk increase, with ammonium nitrogen as the limiting factor.

Conclusions. Combining multiyear and seasonal profiling with regulatory exceedance analysis and cluster typology provides an objective, reproducible screening tool for the Southern Bug Basin. Organic-oxygen loading dominates basin-wide, nutrient enrichment forms a distinct risk pattern in the upper reaches, and mineralization-salinity pollution is spatially localized. The identified priority sites give a scientific basis for optimizing the monitoring network and planning water-protection measures, without substituting for official ecological-status classification.

Introduction

The Southern Bug Basin is a water-management system in which natural seasonality of runoff is combined with anthropogenic pressure from urbanized areas, agricultural landscapes, municipal infrastructure, and recreational use of water resources. For such basins, ecological interpretation of long-term hydrochemical series cannot be limited to describing mean concentrations alone: it requires a combination of regulatory assessment, seasonal profiling, identification of priority indicators, and grouping of monitoring sites according to similarity of hydrochemical conditions. This framework is especially relevant under increased vulnerability of water infrastructure, when state monitoring results should be used not only to describe the current state but also to identify reaches requiring priority control.

Recent Ukrainian studies demonstrate that surface water quality assessment should be linked to the concept of environmental risk. Bezsonnyi and Nekos [1] showed that under military danger the priority pollutants in surface runoff and river waters increasingly include organoleptic indicators and nitrogen-containing compounds that can deteriorate aquatic ecosystems and accelerate eutrophication. Bezsonnyi, Plyatsuk, Ponomarenko, and Tretyakov [2] substantiated the use of entropy-weighted water quality indices, because treating all parameters as equivalent or assigning weights solely by expert judgement may lead to the loss of important information. In the study by Bezsonnyi [3], surface-water risk assessment was related to the frequency of exceedance of maximum permissible concentrations for individual components, which is methodologically close to the present article, where exceedance ratios and violation frequencies are used for screening-based ranking of monitoring sites.

The contemporary international literature confirms that integral water quality indices remain convenient tools for summarizing complex hydrochemical data, but they require transparent selection of parameters, regulatory reference values, and weighting procedures. The critical review by Gupta and Gupta [4] emphasizes the evolution of the Water Quality Index and

methodological limitations related to subjectivity in selecting weights and scales. Reviews by Chidiac et al. [5] and Mogane et al. [6] show that WQI facilitates communication of monitoring results to decision-makers, but different index schemes may classify the same water body differently. Akhtar et al. [7] proposed improving WQI calculation using multi-criteria decision-making, while the review by Muniz and Oliveira-Filho [8] summarizes the use of multivariate statistical analysis in water-quality studies. Accordingly, outdated historical approaches of previous decades were not used in this study; instead, the methodological basis was formed from modern index, factor, and cluster analytics presented in Scopus-indexed publications from 2021–2025.

Empirical studies of river and catchment systems in recent years demonstrate the effectiveness of combining WQI, PCA, cluster analysis, discriminant analysis, and GIS visualization. El Azhari et al. [9] combined WQI, multivariate statistics, and GIS for the Mediterranean Oued Laou watershed, which enabled interpretation of anthropogenic influence and the spatial structure of water quality. Wang et al. [10] applied multivariate statistical techniques to assess water quality in the Yuqiao Reservoir watershed and apportion pollution sources. Yao et al. [11] demonstrated the suitability of hydrochemical analysis, PCA, and clustering for evaluating spatial heterogeneity of waters, while Mammeri et al. [12] used WQI and discriminant analysis to identify indicators responsible for spatial differentiation of surface water quality. For the Rokel River, Barrie et al. [13] combined PCA, WQI, cluster analysis, and ANOVA, which is close to the logic of the present study, where multiyear mean concentrations are considered together with clustering similarity among sites. Gaur et al. [14] demonstrated the potential of combining WQI, hydrogeochemical interpretation, and PCA for surface waters in a mountainous region.

A separate group of recent publications addresses long-term monitoring series, seasonal variability, and selection of priority control reaches. Zhalmagambetova et al. [15] used a ten-year dataset containing 26 chemical components at 26 sites in the Irtysh River Basin and showed

that WQI and multivariate statistics are suitable for identifying zones of priority environmental regulation. Akiner, Chauhan, and Singh [16] combined CCME-WQI, factor analysis, PCA, and cluster analysis for long-term series in the Betwa River Basin, providing a direct methodological analogue for multiyear Southern Bug data. Roy et al. [17] developed a PCA-oriented WQI model for rivers in Dhaka and showed that principal components can reduce subjectivity in parameter selection. Hammoumi et al. [18] confirmed the importance of seasonal data stratification in combination with WQI and PCA. Jo et al. [19] used WQI and multivariate statistical techniques to identify key pollutants in standard watersheds within the TMDL policy framework. Alfaleh, Ben Khedher, and Alvarez-Meza [20] substantiated the potential of entropy-weighted WQI and factor analysis for reducing the subjectivity of index-based assessment.

An important addition to this research direction is the study by Bezsonnyi, Tretyakov, Plyatsuk, Ponomarenko, and Davydova [21], in which an entropy-weighted water quality index was applied to more than 540 state surface-water monitoring sites in Ukraine. The authors revealed pronounced seasonal and spatial heterogeneity in surface water quality: better index values were recorded in winter and spring, whereas the most stressed conditions occurred during low-flow and autumn periods; among the most problematic regions, the Southern Bug Basin was specifically identified.

A closely related and more recent contribution is the basin-scale study by Bezsonnyi [22], which applied the same entropy-weighted approach specifically to the Southern Bug River basin, using hydrochemical observations from 36 monitoring stations for 2020–2024 and twelve water-quality parameters. The author established a pronounced downstream and seasonal gradient of degradation: EWQI values increased from clean conditions (Classes II–III) in the upper reaches near Haivoron and Ladyzhyn to very and extremely polluted conditions (Classes VI–VII, EWQI > 3.0) in the estuarine section near Mykolaiv, with the basin-mean index rising from 1.85 in the cold period to 2.46 in the warm period, a 33% seasonal deterioration confirmed by the Mann–Whitney test ($p < 0.01$). Entropy-weight and principal component analyses identified ammonium (22%), phosphates (18%), and BOD₅ (15%) as the dominant contributors to the index, while k-means clustering delineated four water-quality zones ranging from clean headwaters to a critically polluted estuarine cluster. This study confirms, at the basin scale, the priority role of biogenic and organic pollution already indicated by the nationwide assessment [21] and demonstrates the practical feasibility of combining

entropy weighting, PCA, and clustering for the Southern Bug. At the same time, it relies on a comparatively short five-year record (2020–2024) and does not apply a regulatory exceedance-frequency framework or robust outlier-control standardization, which leaves room for the longer-term, regulation-oriented profiling addressed in the present study.

This directly substantiates the need for a more detailed basin-scale analysis of the Southern Bug that combines seasonality, spatial differentiation, and regulatory interpretation. The European context of such work is framed by studies assessing river ecological status in line with the Water Framework Directive. Naddeo et al. [23], using 34 rivers in the Salerno Province as a case study, demonstrated the practical role of aggregated macro-pollution indicators for evaluating river-water status, while Wuijts et al. [24] emphasized that achieving WFD objectives requires not only monitoring but also cross-sectoral river-basin management. The development of data-driven approaches should also be considered: the review by Zhu et al. [25] shows that machine learning is increasingly used for classification, forecasting, and optimization of water-quality monitoring, whereas Uddin et al. [26] demonstrate that outliers and the quality of input data can affect water categorization in index models. Therefore, long state monitoring series require robust standardization, control of technical extremes, and transparent justification of index classes.

The regulatory and institutional framework of the study is based on the state surface-water monitoring system of Ukraine. The State Water Agency defines it as a system for collecting, processing, summarizing, and analysing information on the condition of water bodies in order to forecast changes and prepare scientifically grounded management recommendations [27]. At the same time, official assignment of surface-water bodies to ecological and chemical status classes is regulated by the Methodology approved by Order No. 5 of the Ministry of Environmental Protection of Ukraine dated 14 January 2019 [28]. This article does not perform full official classification of the ecological status of water bodies, because that procedure requires not only physical-chemical but also biological and hydromorphological indicators. Instead, a screening hydrochemical assessment is applied through the ratio and frequency of exceedance of regulatory reference values formed with due regard to hygienic water-quality standards [29] and methodological recommendations on maximum permissible discharge standards [30]. The European context is set by the EU Water Framework Directive, which establishes the river-basin management principle and the requirement to achieve good water status [31].

Thus, the current state of research indicates five methodological requirements for analysing long-term hydrochemical series. First, results should be interpreted in regulatory terms rather than remain merely statistically descriptive. Second, integral indices should have a transparent formula, an understandable weighting system, or a justified decision not to apply weighting. Third, multivariate statistics should be used to test the internal structure of the data and identify typical profiles. Fourth, seasonality and spatiality should be analysed jointly, because hydrochemical indicators strongly depend on water availability, thermal regime, dilution, and local sources of substance inputs. Fifth, long monitoring series require data-quality control, detection of technical extremes, and robust standardization procedures so that isolated anomalous values do not determine cluster structure or index-based ranking.

For the Southern Bug Basin, such an integrated scheme remains insufficiently represented in the open scientific literature: existing approaches generally either assess individual water-quality indices, apply multivariate statistics without comprehensive regulatory profiling, or consider Ukraine at a generalized inter-basin level. Therefore, combining multiyear mean concentrations, seasonal profiles, ratios of exceedance of regulatory reference values, robust data preparation, PCA visualization, and clustering of monitoring sites provides a justified methodological basis for identifying organic-oxygen, nutrient, and mineralization-salinity profiles within this basin.

The purpose of the study is to perform factor-cluster and regulatory-index profiling of long-term hydrochemical series for rivers of the Southern Bug Basin in order to identify sites dominated by organic, nutrient, or mineralization-salinity pollution and to rank reaches by hydrochemical risk level. The object of the study is surface

waters of rivers in the Southern Bug Basin. The subject of the study is the long-term structure of hydrochemical indicators, their seasonal variability, regulatory exceedances, and cluster profiles of monitoring sites.

Materials and Methods

The analysis was based on processed data from the state surface-water monitoring system of the State Water Agency of Ukraine. From the general dataset, records with Riverbas_Name = “Southern Bug” were selected. The resulting sample contains 5,654 records for 13 January 2003–18 March 2026 from 95 monitoring sites. The analysis included BOD₅, suspended solids, dissolved oxygen, sulphates, chlorides, ammonium nitrogen, nitrates, nitrites, phosphates, surfactants, permanganate oxidizability, COD, atrazine, and simazine. The “total nitrogen” indicator contained no filled values in the selected fragment and was not used in calculations. General principles of handling laboratory-control data, harmonizing measurement units, and ensuring sample traceability were aligned with current standards for hydrochemical analysis and sampling/preservation of water samples [32, 33].

At the stage of physical-chemical plausibility control, 57 obviously technical values were removed at the level of individual data cells. Technical extremes were defined as values exceeding a realistic range for surface waters by one or several orders of magnitude or contradicting the analytical nature of the indicator, including values of approximately 40–45 thousand for indicators originally measured in mg/dm³. For dissolved oxygen, values above 20 mg/dm³ were additionally reviewed as potentially related to data-entry errors, because without accompanying information on temperature, saturation, and measurement methodology they cannot be unambiguously used in index calculations (Table 1).

Table 1

Control of technical extremes in the Southern Bug basin sample

Indicator	Removed values	Minimum removed value	Maximum removed value
BOD ₅	2	44562.0	45323.0
Suspended solids	2	45392.0	45394.0
Dissolved oxygen	25	20.24	45748.0
Sulphates	0	-	-
Chlorides	2	5076.4	5615.3
Ammonium nitrogen	0	-	-
Nitrates	3	45324.0	45383.0
Nitrites	11	10.58	109.0
Phosphates	2	406.0	45474.0
Surfactants	0	-	-
Permanganate oxidizability	7	320.0	43800.0
COD	3	4068.0	45443.0
Atrazine	0	-	-
Simazine	0	-	-

The stability check showed that removal of technical extremes did not change the overall structure of the conclusions: the leading indicator groups, the balance among organic, nutrient, and mineralization-salinity profiles, and the list of priority reaches remained interpretatively stable. General principles of data-quality control and laboratory-analytical reproducibility were aligned with current guidance on water analysis and sample handling [32; 33].

For each site p and indicator j , the multiyear mean concentration was calculated as follows:

$$\bar{C}_{pj} = (1 / npj) \cdot \sum C_{ipj} \quad (1)$$

where $\bar{C}_{pj}$ is the mean concentration of indicator j at site p ;

C_{ipj} is an individual observation;

npj is the number of measurements for the corresponding “site-indicator” pair.

The seasonal profile was calculated separately for winter, spring, summer, and autumn:

$$\bar{C}_{pjs} = (1 / npjs) \cdot \sum C_{ipjs} \quad (2)$$

where s is the season.

This scheme allows winter and summer low-flow periods, spring dilution, and autumn runoff-formation conditions to be distinguished.

Regulatory interpretation was based on the exceedance ratio relative to a regulatory reference value. For indicators for which an increase in concentration is hazardous, the following expression was used:

$$K_{ij} = C_{ij} / N_j \quad (3)$$

where K_{ij} is the exceedance ratio or the degree of approach to the reference value;

C_{ij} is the measured concentration;

N_j is the regulatory value.

For dissolved oxygen, the inverse principle was used: a violation was recorded when concentration was lower than the minimum acceptable reference value.

$$K(O_2) = N_{\min(O_2)} / C(O_2), \text{ if } C(O_2) < N_{\min(O_2)} \quad (4)$$

The violation frequency for indicator j at a site or in the entire basin was determined as:

$$F_j = (m_j / n_j) \cdot 100 \% \quad (5)$$

where m_j is the number of samples with an exceedance/violation of the reference value, and n_j is the number of samples with an available value for the indicator.

For ranking of sites, a modified regulatory index $I6$ was used; it was constructed as the mean of the six highest partial ratios K at a monitoring site:

$$I6p = (1 / 6) \cdot \sum Kp(r), r = 1...6, \\ Kp(r) \text{ are the six highest } K \text{ values at site } p \quad (6)$$

The $I6$ index was used as an author-defined screening tool for ranking sites by hydrochemical risk. It is not an official water-quality index and does not replace the assignment of surface-water bodies to ecological or chemical status classes. In equation (6), $Kp(r)$ denotes the six highest mean partial exceedance ratios for site p across all indicators used; ranking was performed separately for domestic-use and fishery-use reference values. Using the six highest partial ratios prevents risk from being “diluted” by a large number of less relevant indicators while preserving comparability among sites. The following screening classes were used for $I6$: $I \leq 1$ – conditionally low risk; $1 < I \leq 2.5$ – moderate risk; $2.5 < I \leq 4$ – significant risk; $4 < I \leq 6$ – high risk; $I > 6$ – critical risk (Table 2).

All indicators were preliminarily grouped into three analytical blocks: organic-oxygen, nutrient, and mineralization-salinity. Block scores were calculated as mean partial ratios K for the corresponding indicators. This index-cluster logic is consistent with modern approaches that combine WQI, PCA, cluster analysis, and multivariate statistics in hydrochemical studies [8; 15; 16; 17; 18]. To stabilize distributions, a $\log(1 + x)$ transformation was applied, after which the data were scaled robustly using the median and the interquartile range:

$$Z_{ij} = [\log(1 + X_{ij}) - Me_j] / IQR_j \quad (7)$$

where Z_{ij} is the robustly standardized value;

X_{ij} is a block or indicator score;

Me_j is the median;

IQR_j is the interquartile range.

Principal component analysis was used not as a self-sufficient procedure for official water-quality classification, but as a tool for visualizing the variation structure of the three block indicators. Monitoring sites were clustered by the k -means algorithm in the space of organic-oxygen, nutrient, and mineralization-salinity blocks. The objective function of the algorithm is:

$$\arg \min \sum_k \sum_{p \in S_k} ||Z_p - \mu_k||^2 \quad (8)$$

To select the number of clusters, variants $K = 2-5$ were tested. The final decision in favour of $K = 3$ was made not only on the basis of the

Table 2

Regulatory reference values used for screening assessment

Indicator	Analytical block	Domestic-use reference value, mg/dm ³	Fishery-use reference value, mg/dm ³	Use in assessment
BOD5	organic block	≤ 6	≤ 3	direct ratio K = C/N
COD	organic block	≤ 30	≤ 30	direct ratio
Permanganate oxidizability	organic block	≤ 10	≤ 10	direct ratio
Dissolved oxygen	oxygen regime	≥ 4	≥ 6	violation due to oxygen deficit
Ammonium nitrogen	nutrient block	≤ 2.0	≤ 0.5	direct ratio
Nitrates	nutrient block	≤ 45	≤ 40	direct ratio
Nitrites	nutrient block	≤ 3.3	≤ 0.08	direct ratio
Phosphates	nutrient block	≤ 3.5	≤ 2.14	direct ratio
Sulphates	mineralization-salinity block	≤ 500	≤ 100	direct ratio
Chlorides	mineralization-salinity block	≤ 350	≤ 300	direct ratio
Surfactants	additional anthropogenic block	≤ 0.5	≤ 0.1	direct ratio

Note. The regulatory reference values presented here were used only for screening assessment of exceedance ratios and violation frequencies. They are not a procedure for officially assigning surface-water bodies to ecological or chemical status classes. Domestic-use and fishery-use reference values were applied as comparable regulatory thresholds for index-based ranking of sites, while results were interpreted as hydrochemical risk based on physical-chemical indicators.

Table 3

Testing the number of clusters using the silhouette coefficient

K	Silhouette score	Group sizes	Methodological interpretation
2	0.839	46; 2	highest coefficient, but excessive merging of most sites
3	0.583	43; 3; 2	selected as the optimal compromise between statistical quality and ecological interpretability
4	0.388	24; 20; 2; 2	artificial splitting of the baseline organic-oxygen profile
5	0.434	24; 13; 7; 2; 2	formation of unstable small groups and more complicated ecological interpretation

silhouette coefficient, but by combining statistical quality, grouping stability, and ecological interpretability of the profiles (Table 3).

The $K = 2$ variant had the highest silhouette coefficient, but it excessively merged 46 of 48 sites into one class. The $K = 3$ variant retained an acceptable silhouette coefficient of 0.583 and enabled interpretation of three ecologically meaningful profiles: organic-oxygen, nutrient, and mineralization-salinity.

Results

The Southern Bug Basin sample covers 5,654 records and 95 monitoring sites. For regulatory ranking and clustering, 48 sites with sufficient repetition of observations were selected. This approach reduces randomness associated with single or sparse observations and enables representative hydrochemical profiles to be formed.

Regulatory exceedances. Under domestic-use regulatory reference values, exceedances were most frequently found for indicators of the organic block: COD, permanganate oxidizability, and BOD5 (Table 4, Fig. 1).

This indicates that, at the basin scale, the organic-oxygen component is the leading component of hydrochemical pressure. Mineralization-salinity pollution appears more locally, but for certain lower reaches of the Southern Bug and Inhul Rivers it reaches high chloride and sulphate ratios. A graphical summary of these violation frequencies is provided in Fig. 1.

Figure 1 clearly confirms that the largest shares of exceedances are concentrated in indicators of the organic block.

Comparison with fishery-use reference values substantially strengthens the assessment of pressure (Table 5).

The highest shares of violations were found for BOD5, COD, sulphates, permanganate oxidizability, nitrites, and ammonium nitrogen. Thus, for protecting aquatic ecosystems, organic and nutrient loading should be treated as priorities. A visual comparison of violation shares is presented in Fig. 2.

Figure 2 shows that fishery-use regulatory reference values reveal a broader spectrum of problematic indicators than domestic-use reference values.

Table 4

Frequency of exceedance of domestic-use regulatory reference values

Indicator	Reference value	n	Violations	Share, %	Maximum ratio
COD	30.0	4972	2134	42.90	9.390
Permanganate oxidizability	10.0	4017	1640	40.80	7.800
BOD ₅	6.0	4983	735	14.80	8.480
Sulphates	500.0	4893	293	6.000	7.150
Ammonium nitrogen	2.0	4983	179	3.600	19.71
Dissolved oxygen	≥ 4	5183	183	3.500	13.33
Chlorides	350.0	4891	153	3.100	13.60
Phosphates	3.5	4976	32	0.600	3.970
Nitrites	3.3	4971	27	0.500	2.180
Nitrates	45.0	4982	20	0.400	2.960
Surfactants	0.5	4355	8	0.200	2.740

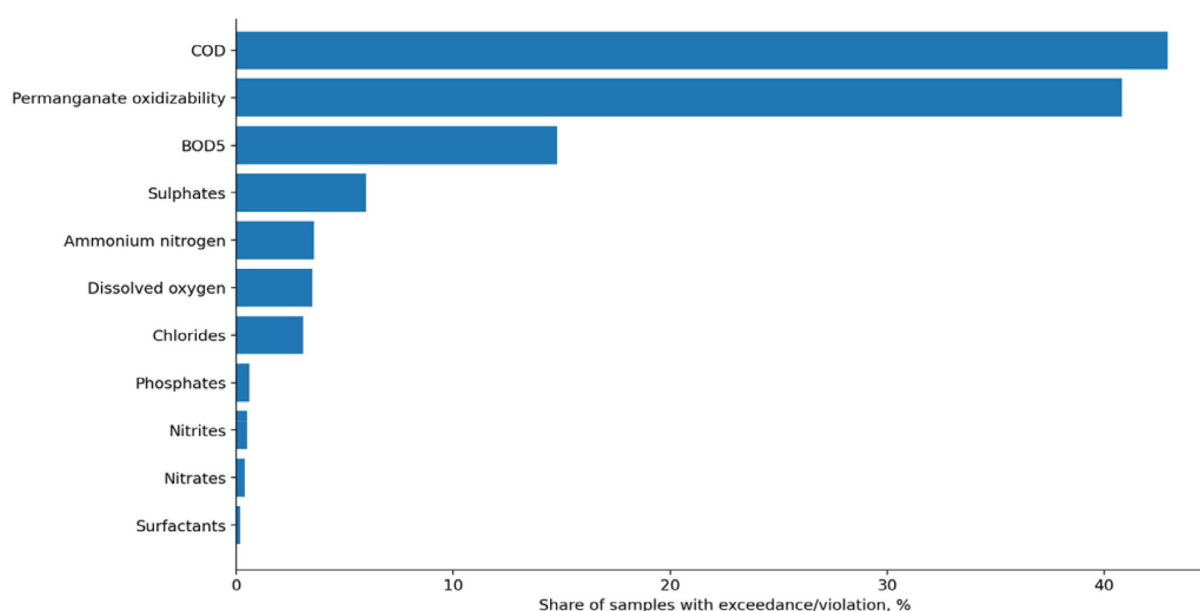


Fig. 1. Share of samples exceeding domestic-use regulatory reference values.

Seasonal hydrochemical profiles. Seasonal analysis shows that the organic block retains an increased role during the warm period, when mean COD and BOD₅ values combine with a decrease in dissolved oxygen concentration (Table 6).

In summer, the mean oxygen concentration was 7.597 mg/dm³ compared with 10.803 mg/dm³ in winter. This is consistent with higher water temperature, intensification of biochemical oxygen demand, and seasonal bioproduction processes. The dynamics of the organic block are shown in Fig. 3.

Table 5

Frequency of exceedance of fishery-use regulatory reference values

Indicator	Reference value	n	Violations	Share, %	Maximum ratio
BOD ₅	3.0	4983	3011	60.40	16.97
COD	30.0	4972	2134	42.90	9.390
Sulphates	100.0	4893	2077	42.40	35.73
Permanganate oxidizability	10.0	4017	1640	40.80	7.800
Nitrites	0.08	4971	1565	31.50	90.00
Ammonium nitrogen	0.5	4983	939	18.80	78.85
Dissolved oxygen	≥ 6	5183	700	13.50	20.00
Surfactants	0.1	4355	267	6.100	13.70
Chlorides	300.0	4891	160	3.300	15.86
Phosphates	2.14	4976	95	1.900	6.490
Nitrates	40.0	4982	35	0.700	3.330

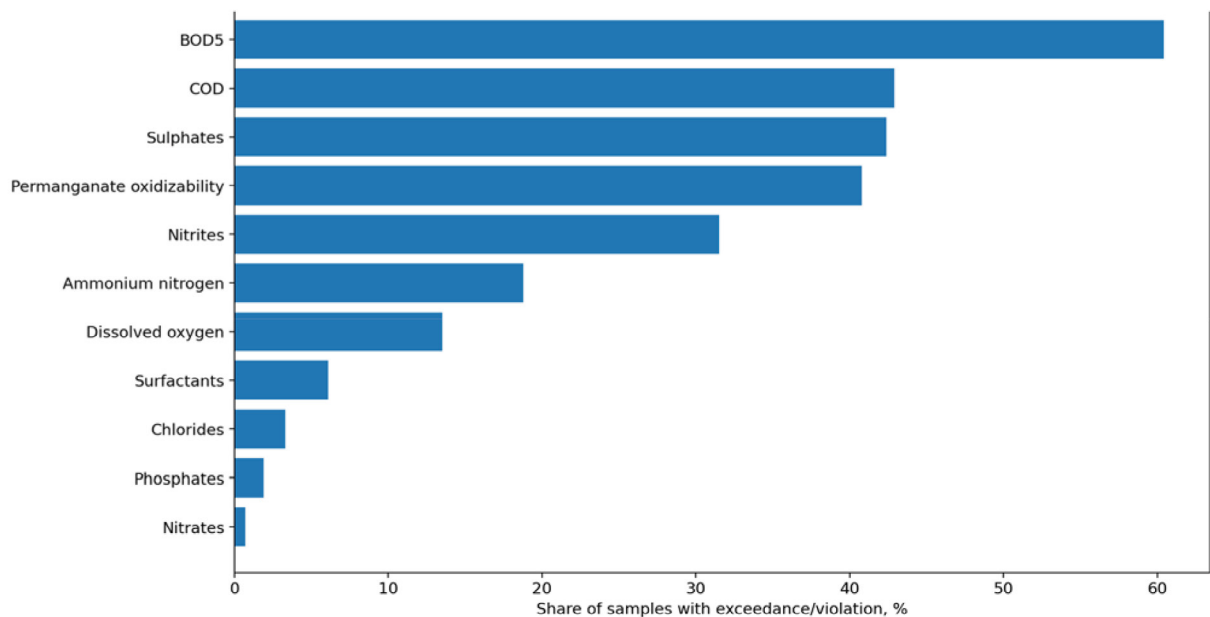


Fig. 2. Share of samples exceeding fishery-use regulatory reference values.

Figure 3 demonstrates higher COD and permanganate oxidizability during the warm period against the background of relatively stable mean BOD5 values.

Seasonal changes in nutrient indicators are shown in Fig. 4.

Figure 4 indicates a marked decrease in nitrates in summer together with a local increase in nitrites and phosphates.

Table 6

Seasonal mean concentrations of the main indicators, mg/dm³

Season	BOD ₅	O ₂	COD	Permang. oxid.	NH ₄	NO ₃	NO ₂	PO ₄	SO ₄	Cl	Surfactants
Winter	3.179	10.80	27.74	9.910	0.559	6.719	0.134	0.425	165.5	102.7	0.037
Spring	4.108	10.16	28.45	11.71	0.551	5.374	0.130	0.289	146.4	90.63	0.042
Summer	4.078	7.597	31.23	11.70	0.512	3.042	0.141	0.552	168.1	107.3	0.042
Autumn	4.025	8.425	30.14	12.71	0.573	3.810	0.193	0.453	155.5	143.6	0.043

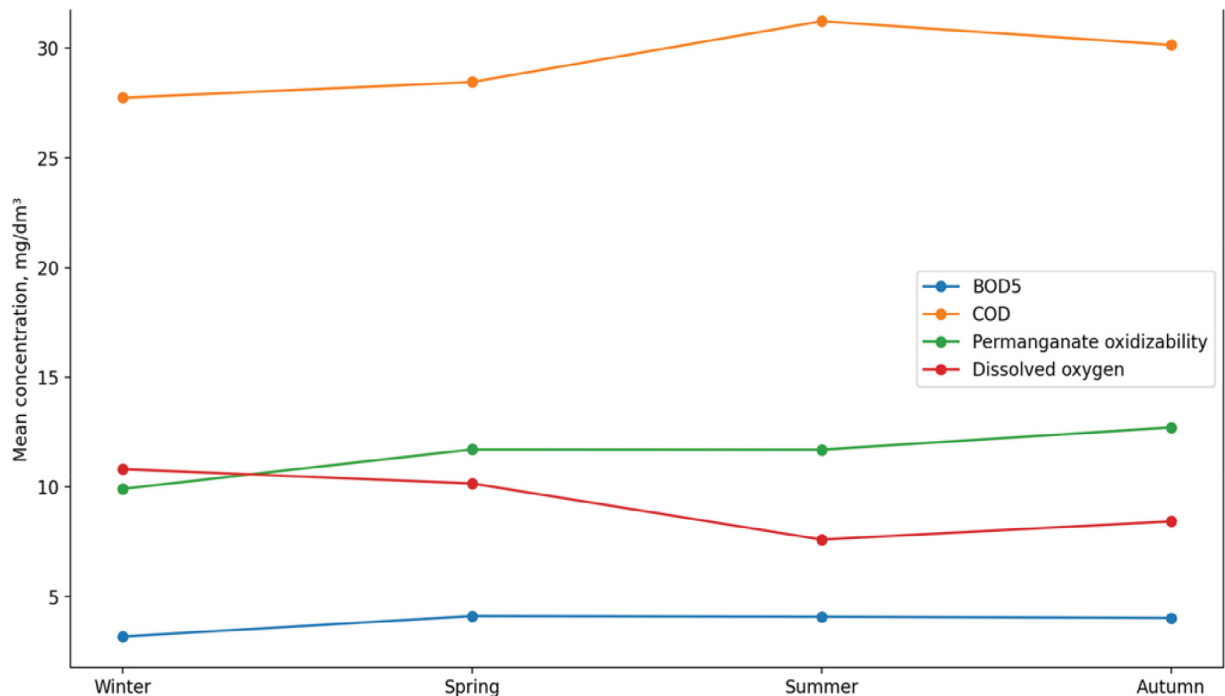


Fig. 3. Seasonal profile of the organic block.

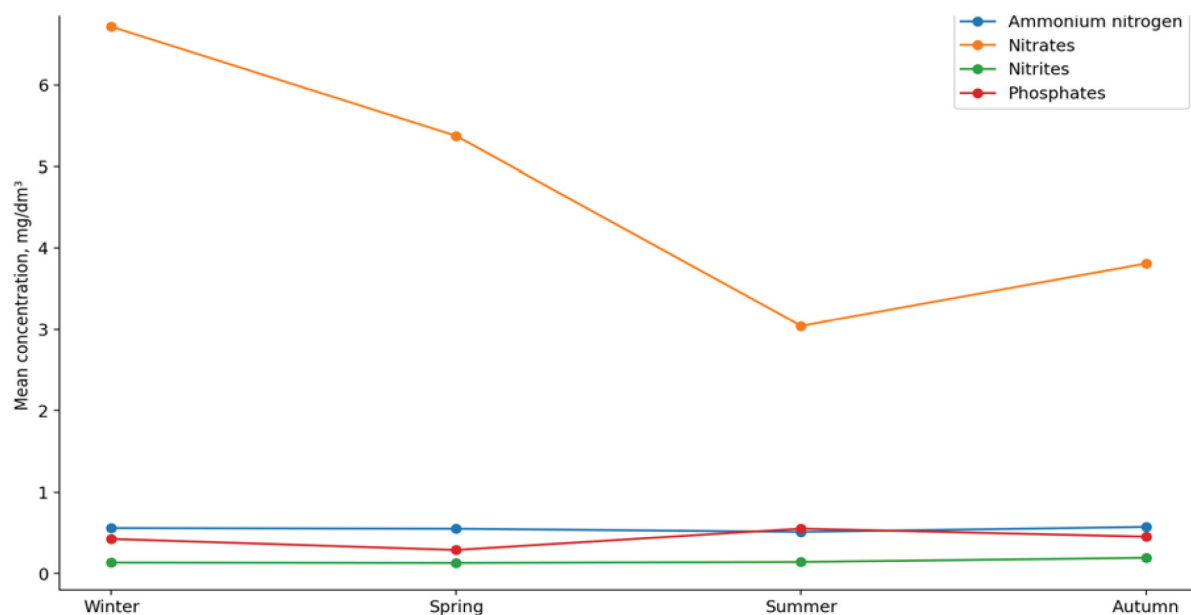


Fig. 4. Seasonal profile of the nutrient block.

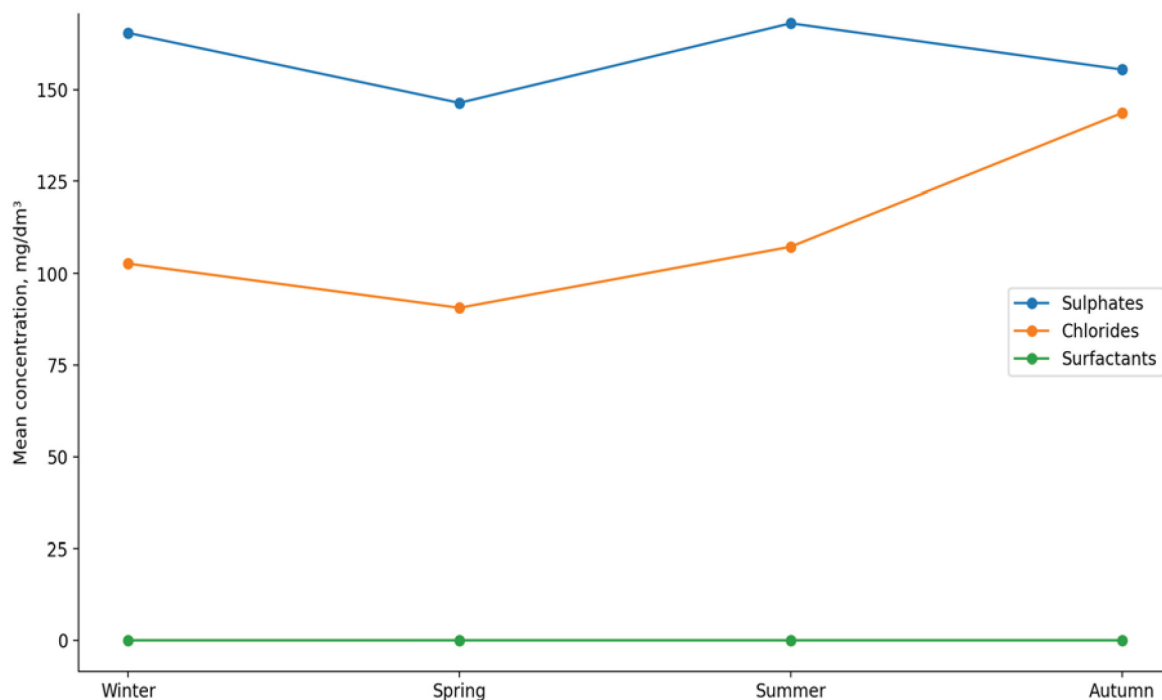


Fig. 5. Seasonal profile of the mineralization-salinity block.

The dynamics of the mineralization-salinity block are presented in Fig. 5.

Figure 5 highlights an increase in chlorides in autumn and relatively high mean sulphate concentrations during the summer period.

PCA visualization in the space of three block scores showed that the first component explains 80.4% of the variation and primarily reflects the nutrient gradient, whereas the second component explains 13.5% and is associated with the mineralization-salinity gradient. This result should not be interpreted as a full official factor classification of water bodies; it was used for graphical confirmation that differentiation among

the most problematic sites is driven primarily by nutrient and salinity components.

Quantitative loadings of the block indicators on the first two principal components are presented in Table 7.

As shown in Table 7, PC1 almost entirely reflects the nutrient block, whereas PC2 is associated with the mineralization-salinity block.

Summary characteristics of the identified cluster profiles are presented in Table 8.

Table 8 shows that the mineralization-salinity profile has the highest mean I6 index, whereas the organic-oxygen profile includes the overwhelming majority of monitoring sites.

Table 7

Loadings of block indicators on principal components

Block	PC1	PC2
Organic-oxygen	0.036	0.102
Nutrient	0.999	0.028
Mineralization-salinity	-0.032	0.994

Table 8

Cluster hydrochemical profiles of monitoring sites

Profile	Number of sites	Mean I6	Mean organic block	Mean nutrient block	Mean mineral block
organic-oxygen profile	43	0.720	0.926	0.102	0.275
mineralization-salinity profile	3	1.561	1.158	0.179	2.318
nutrient profile	2	1.387	0.957	1.246	0.110

Graphical clustering of monitoring sites in the space of block hydrochemical profiles is presented in Fig. 6.

Figure 6 visualizes the separation of two small clusters with distinct nutrient and mineralization-salinity features from the main group of sites.

The spatial positions of the sites belonging to each cluster are shown in Fig. 7.

The organic-oxygen profile includes 43 sites and represents the baseline pressure structure for the basin. The nutrient profile covers two sites in the upper Southern Bug; downstream of Khmelnytskyi and in the Medzhybizh Reservoir area. The mineralization-salinity profile is represented by three sites, including the lower

Southern Bug in the Bug Estuary area, the Inhul River in Mykolaiv, and the Kodyma River near Balta. This structure corresponds to spatial changes in pressure sources: from nutrient influence in upper urbanized reaches to higher mineralization in the lower part of the basin.

The I6 index based on domestic-use reference values showed that most representative sites belong to screening class I, whereas six sites fall into class II, i.e. moderate hydrochemical risk. The highest values were characteristic of the Bug Estuary within Mykolaiv, the lower Inhul River in Mykolaiv, the upper Southern Bug downstream of Khmelnytskyi, the Medzhybizh Reservoir, the Kodyma River near Balta, and

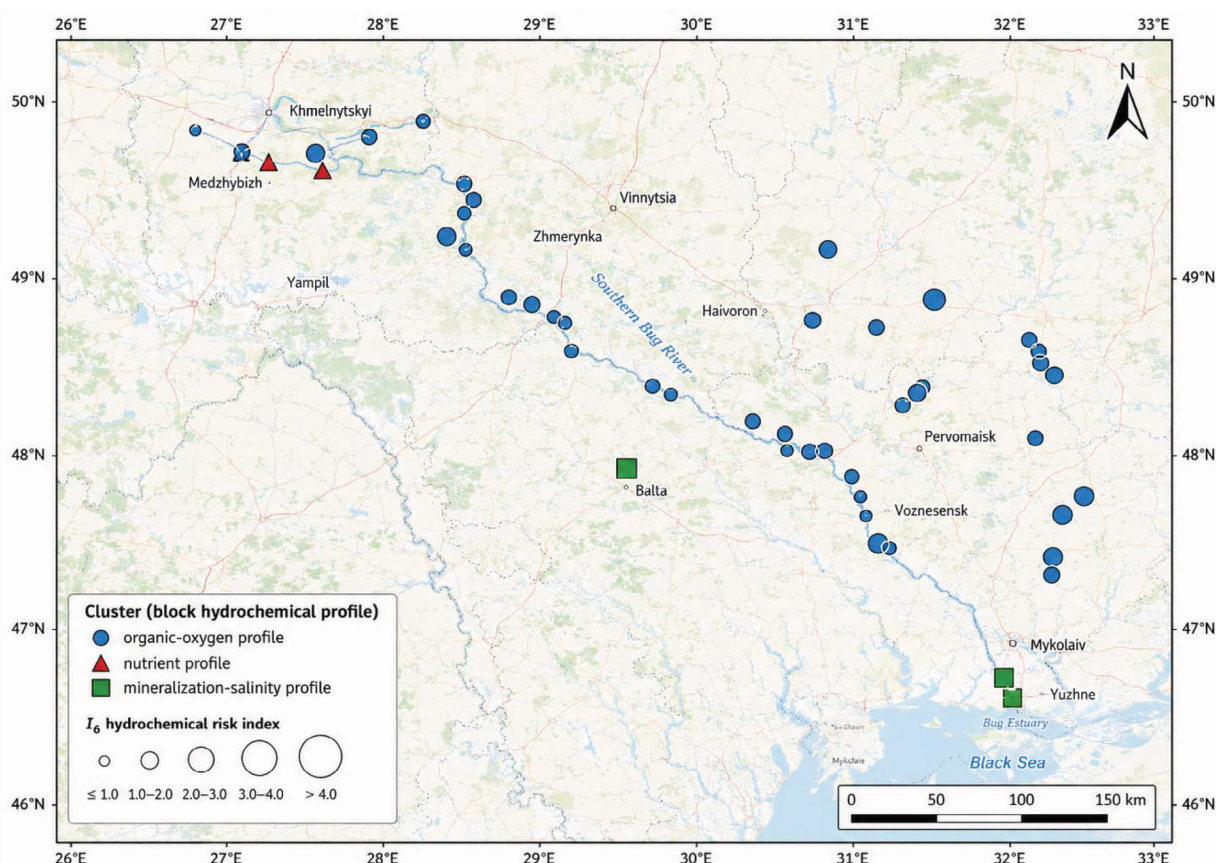


Fig. 6. Clustering of monitoring sites by block hydrochemical profiles.

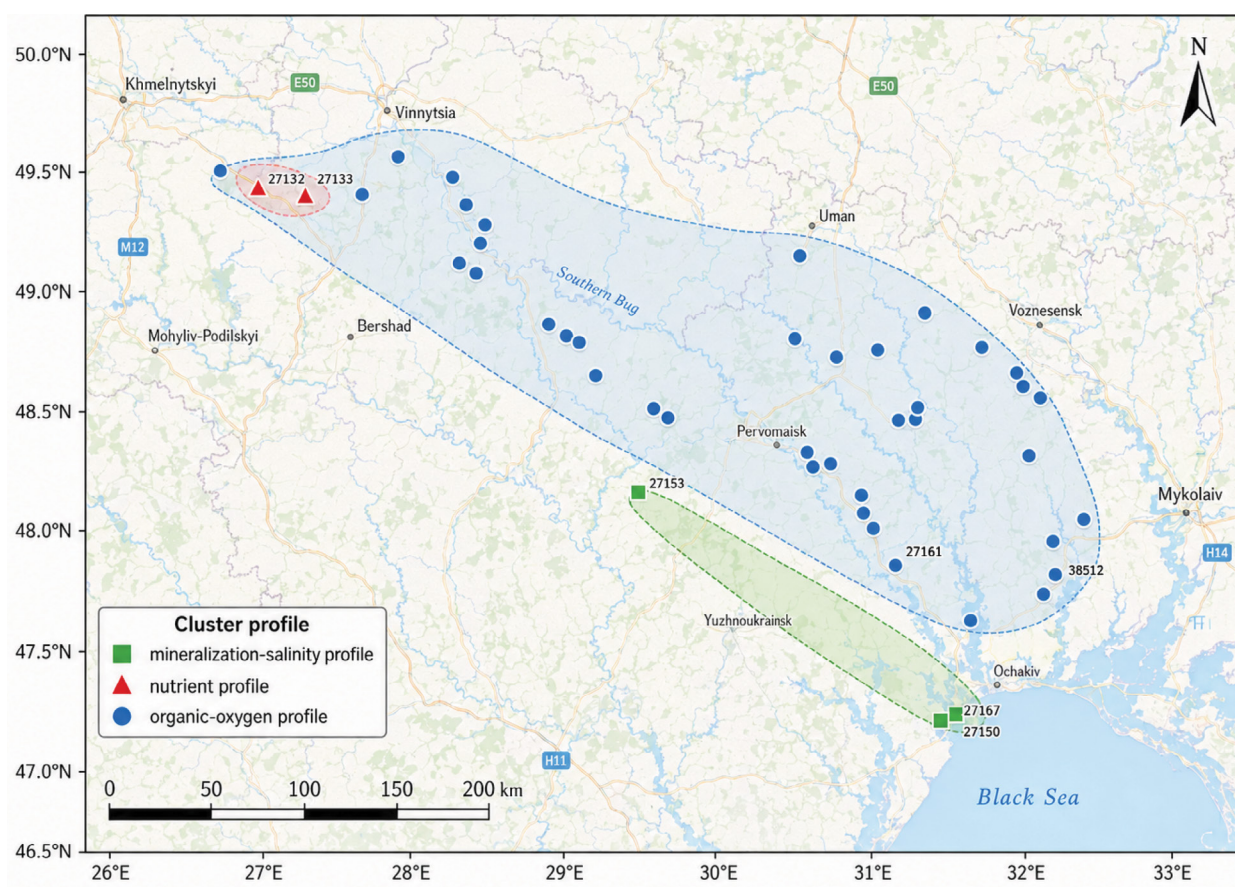


Fig. 7. Spatial scheme of monitoring sites by clusters.

the reach downstream of the discharge of Vinnytsiavodokanal.

Ranking of sites according to domestic-use regulatory reference values is detailed in Table 9.

Table 9 shows that the maximum I6 values are formed both in the lower part of the basin and at selected upper reaches of the Southern Bug.

For a visual comparison of these sites by I6 magnitude, Fig. 8 is used.

Figure 8 confirms that, under domestic-use reference values, differences among the leading sites are moderate, although spatially they cover different parts of the basin.

Under fishery-use reference values, the picture is substantially stricter: one site belongs to screening class V, one to class IV, three to class III, and most problematic reaches move into class II. This demonstrates that ecosystem-oriented

Table 9

Sites with the highest I6 index according to domestic-use reference values

Site ID	Monitoring site	n	I6	Risk class	Limiting indicator	Maximum K
27150	Southern Bug River, 0.5 km, Mykolaiv, Bug Estuary, industrial water intake of Mykolaiv CHP (left part of the seaport)	64	1.852	II – moderate risk	chlorides	6.010
27167	Inhul River, 2 km, Mykolaiv, 2 Naberezhna Street, old pedestrian bridge across the Inhul River	51	1.633	II – moderate risk	chlorides	4.475
27132	Southern Bug River, 744 km, Kopystyn village, downstream of Khmelnytskyi	71	1.555	II – moderate risk	ammonium nitrogen	4.588
27133	Southern Bug River, 711 km, Medzhybizh urban-type settlement, Medzhybizh Reservoir	67	1.219	II – moderate risk	ammonium nitrogen	3.283
27153	Kodyma River, 103 km, Balta, agricultural water intake	80	1.197	II – moderate risk	permanganate oxidizability	2.427
27138	Southern Bug River, 569.5 km, 500 m downstream of the Vinnytsiavodokanal discharge (1.5 km downstream of the Sabariv Reservoir dam)	170	1.014	II – moderate risk	permanganate oxidizability	2.105

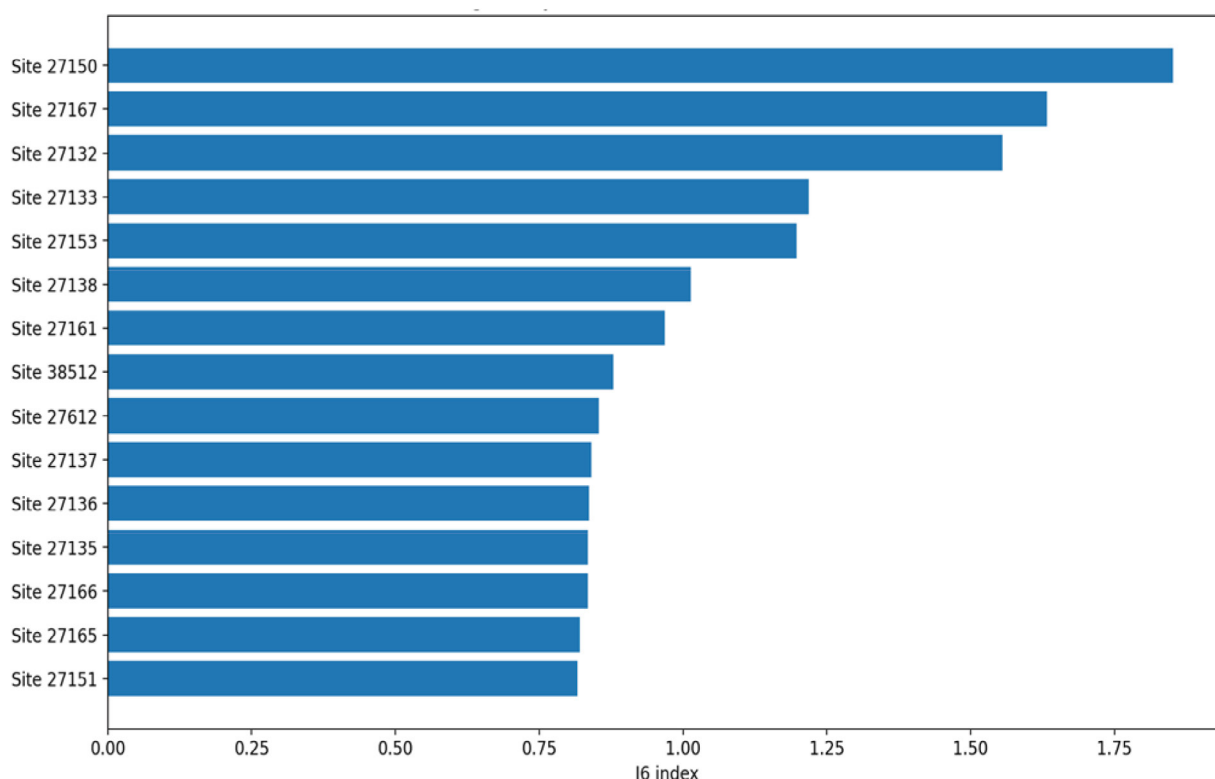


Fig. 8. Sites with the highest hydrochemical risk according to domestic-use reference values.

assessment is more sensitive to nutrient forms of nitrogen, BOD₅, sulphates, and oxygen deficit.

Sites with the highest I6 values under fishery-use reference values are systematized in Table 10.

Table 10 demonstrates a sharp increase in the I6 index in the upper Southern Bug, where ammonium nitrogen acts as the limiting factor.

Graphical ranking of these sites is presented in Fig. 9.

Figure 9 demonstrates that the fishery-use approach substantially increases the contrast between the most problematic and background monitoring sites.

Discussion

The obtained results demonstrate that the long-term monitoring series for the Southern Bug should be interpreted not only through mean concentrations, but through the combined analysis of regulatory exceedance frequency, seasonality, and site typology. If the analysis were limited to mean concentrations alone, some problematic reaches with high exceedance frequencies or high peak ratios would remain insufficiently highlighted. Therefore, the I6 index, which focuses on the six most problematic partial ratios, is a useful screening tool.

Table 10

Sites with the highest I6 index according to fishery-use reference values

Site ID	Monitoring site	n	I6	Risk class	Limiting indicator	Maximum K
27132	Southern Bug River, 744 km, Kopystyn village, downstream of Khmelnytskyi	71	7.003	V – critical risk	ammonium nitrogen	18.35
27133	Southern Bug River, 711 km, Medzhybizh urban-type settlement, Medzhybizh Reservoir	67	4.678	IV – high risk	ammonium nitrogen	13.13
27150	Southern Bug River, 0.5 km, Mykolaiv, Bug Estuary, industrial water intake of Mykolaiv CHP (left part of the seaport)	64	2.743	III – significant risk	chlorides	7.011
27153	Kodyma River, 103 km, Balta, agricultural water intake	80	2.694	III – significant risk	nitrites	6.773
27138	Southern Bug River, 569.5 km, 500 m downstream of the Vinnytsiavodokanal discharge (1.5 km downstream of the Sabariv Reservoir dam)	170	2.539	III – significant risk	nitrites	6.681

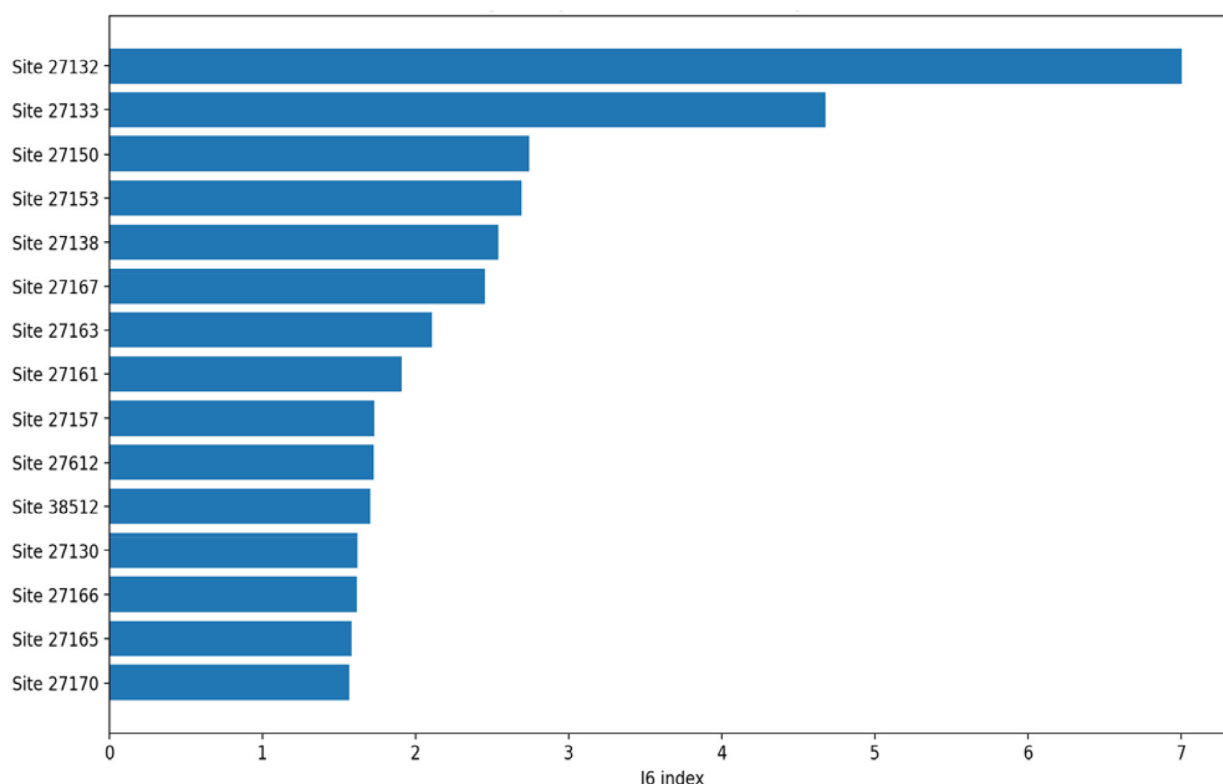


Fig. 9. Sites with the highest hydrochemical risk according to fishery-use reference values.

Dominance of the organic-oxygen profile at most sites does not imply the same state for the entire basin system. On the contrary, this result should be interpreted as a background structural feature of long-term hydrochemical data, onto which nutrient or mineralization-salinity deviations are locally superimposed. For reaches downstream of large settlements, increased BOD₅, COD, permanganate oxidizability, and nitrogen forms are logical. For the lower part of the basin and estuarine zone, a stronger role of chlorides and sulphates is expected and may be associated with both natural-hydrological and anthropogenic factors.

The nutrient profile identified for upper Southern Bug sites has particular ecological significance. Increased ammonium nitrogen, nitrites, and phosphates may act as preconditions for eutrophication, deterioration of oxygen regime, and changes in biotic condition. In this respect, the results are consistent with previous studies in which nitrogen-containing substances were considered priority pollutants under increased environmental risk.

Comparison of domestic-use and fishery-use reference values reveals a methodologically important difference. Under domestic-use reference values, a substantial share of sites has low or moderate screening risk. Under fishery-use reference values, the picture is considerably more stressed, because aquatic ecosystems are more sensitive to organic loading, oxygen deficit,

nitrites, ammonium, and sulphates. Therefore, for environmental planning, both scales should be presented: the first characterizes the sanitary and household dimension, whereas the second reflects ecosystem vulnerability.

The applied methodology has several limitations. First, it does not replace the official ecological-status classification of surface-water bodies, because it does not include the full set of biological, hydromorphological, and priority chemical indicators. Second, state monitoring series have unequal repetition across sites and indicators, so only sites with a sufficient number of observations were selected for clustering. Third, the absence of discharge data and information on specific effluent releases does not allow the analysis to move from hydrochemical profiling to a full calculation of assimilative capacity or maximum permissible discharge. Fourth, technical extremes were removed at the level of individual values rather than entire samples; this minimizes information loss but requires preservation of the data-cleaning protocol in supplementary materials. At the same time, the stability check confirmed that the main cluster structure and the list of priority reaches do not depend on isolated obvious technical values. The resulting scheme is suitable for preliminary identification of reaches that require further detail in state monitoring programmes and river-basin management plans.

Conclusions

Based on processed state monitoring data for 2003–2026, 5,654 records from 95 monitoring sites were analysed for the Southern Bug Basin. After physical-chemical plausibility control, 57 obviously technical values were removed, which increased the reliability of mean, index-based, and cluster calculations.

Under domestic-use reference values, the most frequent exceedances were identified for COD (42.9% of samples), permanganate oxidizability (40.8%), and BOD₅ (14.8%), indicating the leading role of organic loading in the overall structure of the basin hydrochemical profile.

Under fishery-use reference values, violation frequencies increase substantially: BOD₅ – 60.4%, COD – 42.9%, sulphates – 42.4%, permanganate oxidizability – 40.8%, nitrites – 31.5%, and ammonium nitrogen – 18.8%. This confirms the higher sensitivity of ecosystem-oriented assessment to nutrient and organic pressure.

Seasonal profiles demonstrate a combination of increased organic indicators during the warm period with decreased dissolved oxygen. The summer mean oxygen concentration is lower than

the winter mean, indicating seasonal stress of the oxygen regime.

Clustering of 48 representative sites, justified by testing $K = 2-5$ using the silhouette coefficient and ecological interpretability, identified three types of hydrochemical profiles: organic-oxygen (43 sites), mineralization-salinity (3 sites), and nutrient (2 sites). The organic-oxygen profile should be interpreted as a baseline structural feature of basin hydrochemical data rather than as uniformly high pollution at all sites in this group.

The modified regulatory index I₆ enabled ranking of sites by hydrochemical risk. Under domestic-use reference values, the highest values were found for the Bug Estuary in Mykolaiv, the lower Inhul River in Mykolaiv, the upper Southern Bug downstream of Khmelnytskyi, the Medzhybizh Reservoir, the Kodyma River near Balta, and the reach downstream of the Vinnytsiavodokanal discharge.

The proposed scheme is a screening tool and does not substitute for official assignment of surface-water bodies to ecological-status classes. It is appropriate for identifying priority reaches for enhanced control, optimizing monitoring programmes, and preparing water-protection measures in the Southern Bug Basin.

Внесок авторів: всі автори зробили рівний внесок у цю роботу

Конфлікт інтересів: автори засвідчують, що, незважаючи на те, що один із авторів статті є членом редакційної колегії цього журналу, процес рецензування, прийняття рішення щодо публікації та редагування проводилися незалежно, без його участі чи впливу. Будь-які потенційні конфлікти інтересів були повністю усунені шляхом зовнішнього контролю процесу.

Декларація про використання генеративного штучного інтелекту: Автори використовували інструменти генеративного штучного інтелекту (GenAI) для допоміжної роботи: моделі ChatGPT-5.5 (OpenAI, 2026) виключно для мовного редагування, структурного впорядкування тексту; Grammarly – для перевірки правильності перекладу тексту, а також для виправлення граматичних та стилістичних помилок. Усі результати роботи з цими інструментами були ретельно контрольовані, перевірені та, за необхідності, відредаговані авторами. Весь науковий контент, матеріали та висновки були створені авторами. Автори несуть повну відповідальність за зміст та цілісність публікації.

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Conflict of Interest: The authors certify that, although one of the authors of the article is a member of the editorial board of this journal, the peer review, publication decision, and editorial processes were conducted independently, without their participation or influence. Any potential conflicts of interest were fully mitigated through external oversight of the process.

Declaration of use of generative artificial intelligence: The authors utilized generative artificial intelligence (GenAI) tools in a supportive capacity: the ChatGPT-5.5 model (OpenAI, 2026) exclusively for language editing and structural text organization; Grammarly – to verify the correctness of the text translation, as well as to correct grammatical and stylistic errors. All outputs from these tools were carefully supervised, reviewed, and, where necessary, edited by the authors. All scientific content, materials, and conclusions were created by the authors. The authors retain full responsibility for the content and integrity of the publication.

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АНОТАЦІЯ

Метою дослідження є факторно-кластерне та нормативно-індексне профілювання багаторічних гідрохімічних рядів річок басейну Південного Бугу для виділення ділянок із домінуванням органічного, біогенного або мінералізаційно-сольового забруднення та ранжування пунктів державного моніторингу за рівнем гідрохімічного ризику. Вихідною базою стали оброблені дані державного моніторингу поверхневих вод Держводагентства за 2003–2026 рр. Використано розрахунок середніх багаторічних концентрацій, сезонних профілів, частоти та кратності перевищення нормативних орієнтирів, модифікований нормативний індекс І6, аналіз головних компонент і кластеризацію за блоковими гідрохімічними профілями. Методична схема адаптує сучасний індексно-факторно-кластерний підхід до умов багаторічних моніторингових рядів. У межах басейну Південного Бугу відібрано 5654 записи з 95 пунктів спостережень за період з 13.01.2003 до 18.03.2026. Після контролю фізико-хімічної правдоподібності вилучено 57 очевидно технічних значень. За господарсько-побутовими орієнтирами найчастіше перевищення встановлено для ХСК (42,9 % проб), перманганатної окиснюваності (40,8 %) і БСК5 (14,8 %). За рибогосподарськими орієнтирами найбільш проблемними є БСК5 (60,4 %), ХСК (42,9 %), сульфати (42,4 %), перманганатна окиснюваність (40,8 %), нітрити (31,5 %) та амонійний азот (18,8 %). Кластеризація 48 репрезентативних пунктів виділила органічно-кисневий профіль (43 пункти), мінералізаційно-сольовий профіль (3 пункти) та біогенний профіль (2 пункти). Найвищий нормативний індекс І6 за господарсько-побутовими орієнтирами характерний для нижньої частини Південного Бугу в районі Бузького лиману, р. Інгул у м. Миколаїв, а також верхніх ділянок Південного Бугу нижче м. Хмельницький. Наукова новизна полягає у поєднанні багаторічного басейнового профілювання з нормативною інтерпретацією частоти перевищень і індексним ранжуванням пунктів моніторингу. Практичне значення результатів полягає у визначенні пріоритетних ділянок для поглибленого контролю, уточнення програм моніторингу та планування водоохоронних заходів.

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