

Original Research

Long-Term Assessment of Water Quality Index Performance in Three Contrasting River Basins of Lithuania

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Abstract

The Water Quality Index (WQI) is widely applied for long-term monitoring and inter-basin comparison of surface water quality; however, its interpretation may vary depending on basin characteristics and hydrological organization. This study evaluates WQI behaviour in three Lithuanian river basins (Nemunas, Mūša, and Venta) representing contrasting spatial scales and hydrological integration during 2001-2024.

Annual monitoring data of key physicochemical parameters were analysed using variability metrics and principal component analysis (PCA) to assess the relationship between WQI and dominant hydrochemical gradients. Although mean WQI levels were similar among basins, marked differences in structural variability were observed. In the large, hydrologically integrated Nemunas basin, the first principal component explained 44.8% of total variance, indicating stronger dimensional consolidation. Smaller basins exhibited more fragmented multidimensional organization. The correlation between WQI and the dominant gradient ranged from strong ($|r| = 0.82-0.86$) in the Nemunas and Mūša basins to moderate ($|r| = 0.40$) in the Venta basin. Significant hydrological control of the primary gradient was detected only in the largest basin ($\rho = -0.48$, $p = 0.001$).

These findings demonstrate that WQI performance is conditioned by basin-scale structural organization. Integrating composite indices with multivariate analysis enhances the interpretation of long-term monitoring data and supports more reliable inter-basin comparisons.

Keywords: Water Quality Index, long-term monitoring, river basins, principal component analysis, hydrological variability

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Introduction

Long-term river monitoring programs generate extensive hydrochemical datasets that support environmental assessment and water management planning. To simplify complex multidimensional information, water quality parameters are frequently aggregated into composite indicators, most commonly the Water Quality Index (WQI). Such indices are widely used for inter-basin comparisons, temporal trend analysis, and ecological status reporting within European and global regulatory frameworks [1-5].

The WQI integrates multiple physicochemical parameters through weighting and aggregation procedures, enabling communication of overall water quality status in a simplified form. Comprehensive methodological reviews have documented the evolution of WQI formulations, weighting strategies, and aggregation approaches, emphasizing both their practical utility and inherent structural limitations [6, 7]. However, aggregation inevitably reduces multidimensional information and may compress variability, influencing how underlying hydrochemical relationships are represented. Previous studies have shown that parameter selection and weighting schemes can affect WQI classification outcomes [8-10]. Multimetric index applications further demonstrate that physicochemical parameter behaviour and index construction choices may substantially influence assessment results [11].

River basins differ in spatial scale, hydrological integration, land-use structure, and dominant pollution sources. Large, hydrologically integrated systems may exhibit partial homogenization of water quality signals due to cumulative loading and mixing processes, whereas smaller or fragmented basins may display stronger localized variability and episodic responses [12, 13]. Long-term spatio-temporal analyses have demonstrated that structural variability may differ considerably within large hydrological systems [14]. Spatial modelling and geostatistical investigations further indicate that pollution gradients and dominant hydrochemical patterns are not uniformly expressed across river networks [15, 16].

Although numerous studies apply WQI for classification and trend assessment, most focus primarily on status determination rather than on evaluating the structural fidelity of the index in representing dominant hydrochemical gradients. Comparative assessment of WQI performance using consistent methodological conditions across basins with contrasting hydrological organization remains limited. In particular, empirical evidence on how composite index behaviour varies as a function of basin-scale structural integration is still insufficient.

Principal component analysis (PCA) is commonly applied to identify dominant gradients in water quality datasets and to explore relationships among parameters [17, 18]. Combining WQI with multivariate analysis

makes it possible to assess not only index levels but also how closely the index reflects the main patterns of hydrochemical variability. However, systematic evaluation of WQI-gradient correspondence across basins differing in spatial and hydrological structure using long-term monitoring data remains scarce.

The present study addresses this methodological gap by evaluating whether identically constructed WQI values exhibit consistent structural correspondence with dominant hydrochemical gradients across river basins differing in spatial scale and hydrological integration. Using long-term monitoring data (2001-2024) from three Lithuanian river basins representing contrasting hydrological organization, the study integrates composite index assessment with multivariate dimensional analysis under consistent methodological conditions.

By providing a structural perspective on WQI interpretation beyond conventional classification-focused applications, this study contributes to the methodological understanding of composite water quality indices and their scale-dependent performance in river basin assessment.

Materials and Methods

Study Area and Monitoring Framework

The study was based on long-term surface water monitoring data from three Lithuanian river basins representing contrasting spatial scales and hydrological integration: Nemunas, Mūša, and Venta. The Nemunas basin is a large, hydrologically integrated system, whereas Mūša represents a smaller and more fragmented basin. Venta is intermediate in terms of drainage area and hydrological consolidation.

Data were obtained from the national surface water quality monitoring network for 2001-2024. Seven stations with complete long-term records were selected (Nemunas: 2; Mūša: 3; Venta: 2). Annual mean concentrations were calculated to focus on long-term variability. Years with missing values for more than one parameter were excluded from WQI calculations.

Water Quality Parameters

The analysis included total phosphorus (TP), nitrate nitrogen (NO_3^- -N), ammonium nitrogen (NH_4^+ -N), biochemical oxygen demand (BOD_7), chemical oxygen demand (CODCr), dissolved oxygen (DO), and pH. These parameters represent nutrient enrichment, organic pollution, and oxygen regime, and are commonly used in river water quality assessment.

Water Quality Index (WQI)

Surface water quality was assessed using the weighted arithmetic Water Quality Index (WQI), following the classical formulation of Brown et al. [19]:

$$WQI = \frac{\sum_{i=1}^n Qi \cdot Wi}{\sum_{i=1}^n Wi} \quad (1)$$

where Qi is the quality rating of parameter i , and Wi is the relative weight assigned to parameter i .

Quality ratings were calculated based on the ratio between observed annual mean concentrations and standard permissible values:

$$Qi = 100 \cdot \frac{Vi - Vo}{Si - Vo} \quad (2)$$

where Vi is the annual mean concentration of parameter i , Vo is the ideal value of the parameter, and Si is the standard permissible value of parameter i .

The ideal value for dissolved oxygen (14.6 mg O₂ L⁻¹) corresponds to theoretical saturation under standard conditions and follows the classical WQI formulation.

When necessary, quality ratings exceeding 100 were truncated to maintain consistent index scaling and interpretability, as values above 100 represent an exceedance of standard limits rather than proportional deterioration beyond the classification range. This procedure does not affect relative variability patterns but prevents disproportionate influence of extreme observations on the aggregated index.

Standard permissible values were adopted from Lithuanian national water quality standards corresponding to good ecological status (Class II). The calculated weights (Wi) and applied values are presented in Table 1.

For dissolved oxygen, the standard value (Si) represents the minimum acceptable concentration for good ecological status.

Statistical and Multivariate Analysis

Differences in WQI among basins were assessed using the Kruskal–Wallis test with post hoc Wilcoxon comparisons. Temporal trends were evaluated using the Mann–Kendall test.

Principal component analysis (PCA) was applied to standardized physicochemical data to identify dominant hydrochemical gradients. Analyses were performed for

pooled and basin-specific datasets. The first principal component (PC1) was interpreted as the dominant gradient. Structural correspondence between WQI and PC1 was evaluated using Pearson correlation (absolute $|r|$ values).

To assess potential hierarchical effects, additional analyses were conducted using basin-averaged annual values. Hydrological influence was examined using Spearman correlation between PC1 scores and annual mean discharge.

Robustness of WQI–PC1 relationships was evaluated using bootstrap resampling (1000 iterations per basin). An equal-weight scenario was additionally tested to assess sensitivity to weighting. All analyses were conducted in R ($p < 0.05$).

Results and Discussion

Inter-Basin Differences In WQI Level and Variability

WQI values differed among the studied river basins in terms of both mean level and variability (Table 2). The highest mean WQI was observed in the Mūša basin, whereas the lowest was recorded in the Venta basin.

Substantial differences were observed in relative variability. The coefficient of variation (CV) was highest in the Mūša basin (0.87), intermediate in the Venta basin (0.64), and lowest in the Nemunas basin (0.17). This indicates that WQI variability in the Mūša basin was approximately five times greater than in the Nemunas basin, despite the absence of statistically significant differences in mean WQI values between these two systems.

The distribution of WQI values differed among the basins (Fig. 1). The Mūša basin exhibited the widest range of values and the greatest dispersion, whereas WQI values in the Nemunas basin were considerably more compact.

The Kruskal–Wallis test indicated statistically significant differences in WQI among basins ($\chi^2 = 21.83$, $p < 0.001$). Pairwise comparisons showed that the Venta basin differed significantly from both the Mūša and

Table 1. Standard permissible values (Si), ideal values (Vo), and calculated weights (Wi) applied in the WQI calculation

Parameter	Unit	Si	Vo	Wi
pH	–	7.5	7.0	0.024
Dissolved Oxygen (DO)	mg O ₂ L ⁻¹	7.0	14.6	0.026
Biochemical Oxygen Demand (BOD ₇)	mg O ₂ L ⁻¹	5.0	0	0.036
Chemical Oxygen Demand (CODCr)	mg O ₂ L ⁻¹	25.0	0	0.007
Nitrate Nitrogen (NO ₃ –N)	mg N L ⁻¹	2.0	0	0.089
Ammonium Nitrogen (NH ₄ ⁺ –N)	mg N L ⁻¹	0.5	0	0.357
Total Phosphorus (TP)	mg P L ⁻¹	0.4	0	0.446

Table 2. Mean and standard deviation of WQI in the studied river basins.

Basin	Mean WQI	SD
Mūša	67.9	59.1
Nemunas	45.5	7.84
Venta	41.8	26.9

Nemunas basins ($p < 0.001$). No statistically significant difference was detected between the Mūša and Nemunas basins ($p > 0.05$). Thus, the primary difference between these two systems concerned variability rather than the mean level. These results indicate that inter-basin differences in WQI are primarily driven by the distinct behaviour of the Venta basin, whereas the Mūša and Nemunas basins exhibit comparable mean conditions, with differences mainly reflected in variability rather than central tendency.

Temporal Dynamics of WQI

During the period 2001-2024, annual mean WQI values in the Nemunas and Venta basins remained relatively stable, without abrupt fluctuations (Fig. 2). In contrast, the Mūša basin exhibited markedly elevated WQI values during 2001-2005, which substantially contributed to the overall variability observed in this system. After this period, WQI values declined and subsequently stabilized.

The Mann–Kendall test indicated a statistically significant decreasing trend in WQI in the Nemunas basin ($\tau = -0.254$, $p = 0.011$), reflecting a long-term decline of the index during the study period.

In the Mūša basin, a negative trend was also observed ($\tau = -0.155$), although it did not reach statistical significance ($p = 0.055$).

No significant trend was detected in the Venta basin ($\tau = -0.020$, $p = 0.852$). These results suggest that long-term WQI dynamics differ among basins, with a clear improving trend in the hydrologically integrated Nemunas system, while smaller basins exhibit weaker or absent trends, reflecting more variable or locally controlled conditions.

Multivariate Hydrochemical Structure (Overall PCA)

Principal component analysis (PCA) of the combined dataset showed that the first principal component (PC1) explained 30.6% of the total variance, while the second component (PC2) accounted for 22.9%. Together, the first two components explained 53.5% of the total variance.

The highest loadings on PC1 were observed for NO_3^- -N (-0.52), DO (0.47), and BOD_7 (0.37), with notable contributions also from NH_4^+ -N and TP (Table 3). PC2 explained an additional 22.9% of the variance.

These results indicate that PC1 represents the dominant hydrochemical gradient in the dataset, while a substantial proportion of variability is distributed across additional dimensions.

Clear differences among river basins were observed in the PCA ordination space (Fig. 3). The Nemunas basin showed a more compact distribution of observations with lower dispersion. In contrast, the Mūša basin exhibited a wider spread of data points, indicating greater variability of physicochemical parameters. The Venta basin occupied an intermediate position between these two systems. This pattern suggests that hydrological integration is associated with the organization of hydrochemical variability, with the Nemunas basin showing a more consolidated structure, while the Mūša basin reflects more heterogeneous and locally driven conditions.

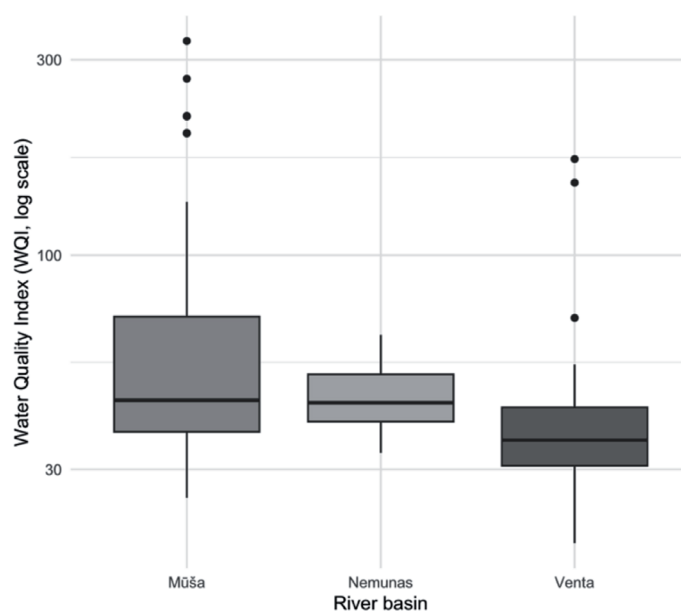


Fig. 1. Distribution of Water Quality Index (WQI) values across the studied river basins.

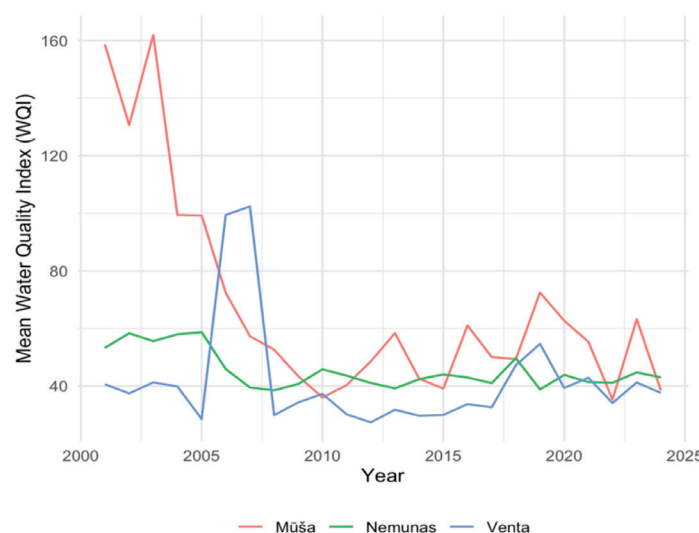


Fig. 2. Inter-annual variation of mean WQI across the Nemunas, Mūša, and Venta river basins.

A moderate negative correlation was observed between WQI and PC1 ($r = -0.55$). The coefficient of determination ($R^2 \approx 0.30$) indicates that approximately 30% of the variability in PC1 scores was associated with WQI values.

This result suggests that WQI reflects the dominant hydrochemical gradient to a certain extent, while a substantial proportion of multivariate variability remains outside the aggregated index. The lower correlation observed in the pooled dataset compared to basin-specific analyses likely reflects structural heterogeneity among basins, where differences in dominant gradient composition and system-specific variability partially attenuate the overall association.

Scale-Dependent Structural Organization

Principal component analysis performed separately for each basin revealed differences in the distribution of explained variance (Fig. 4). In the Nemunas basin, the first principal component (PC1) explained 44.8% of the

total variance, whereas in the Mūša and Venta basins, PC1 accounted for 27.2% and 29.9%, respectively.

These results indicate a higher concentration of variability along the primary gradient in the Nemunas basin compared to the smaller systems. This interpretation reflects a relative concentration of multivariate variance rather than direct proof of process homogenization and should be understood as a structural indication inferred from dimensional organization.

Greater concentration of variance along the first principal component in the Nemunas basin indicates that a larger proportion of total variability was aligned with a single dominant gradient. In contrast, in the Mūša and Venta basins, variability was distributed more evenly across multiple components.

Cumulative variance analysis further illustrated this difference. In the Nemunas basin, the first two principal components explained 64.1% of the total variance, whereas in the Mūša and Venta basins, the first two components accounted for 49.1% and 48.9%, respectively. In the latter basins, approximately 65% of the total variance was reached only after inclusion of the third principal component.

The composition of PC1 also differed among basins (Fig. 5). In the Mūša basin, PC1 was primarily associated with NH_4^+-N and TP (negative loadings). In the Nemunas basin, the dominant gradient included DO, BOD_7 , and TP. In the Venta basin, PC1 was most strongly associated with NO_3^--N and DO.

These differences indicate that the composition of the dominant hydrochemical gradient varied among basins.

To evaluate the relationship between WQI and the primary gradient, Pearson correlation analysis was performed between WQI values and PC1 scores (Table 4). Strong correlations were observed in the Nemunas ($r = 0.82$; $p < 0.001$) and Mūša ($r = -0.86$; $p < 0.001$) basins. In contrast, the Venta basin showed a moderate correlation ($r = -0.40$; $p = 0.004$).

Table 3. Loadings of water quality variables on the first two principal components.

Parameter	PC1	PC2
pH	0.25	-0.16
DO	0.47	-0.23
BOD_7	0.37	-0.43
CODCr	-0.28	-0.03
NO_3^--N	-0.52	0.19
NH_4^+-N	-0.35	-0.58
TP	-0.32	-0.60

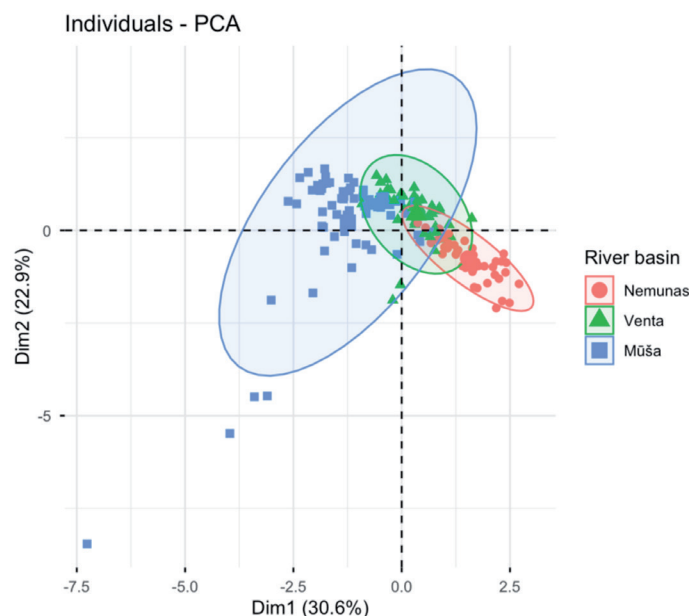


Fig. 3. Principal Component Analysis (PCA) of water quality parameters in the Nemunas, Venta, and Mūša river basins. Ellipses represent 95% confidence intervals.

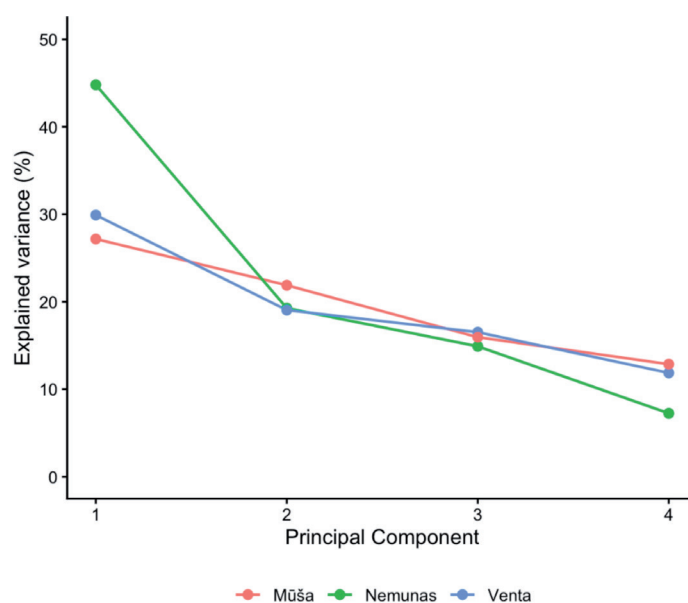


Fig. 4. Explained variance of the first four principal components in the Nemunas, Mūša, and Venta basins.

Differences in the sign of the correlation reflect the arbitrary orientation of PCA components rather than differences in the strength of association.

This suggests that WQI more reliably represents the dominant hydrochemical gradient in structurally simpler or more integrated systems, whereas in the Venta basin, the index captures only part of the underlying multivariate variability.

Hydrological influence was further evaluated using Spearman correlation analysis (Table 5). In the Nemunas basin, a statistically significant negative correlation was detected between PC1 scores and river discharge ($\rho =$

-0.48 ; $p = 0.001$). In contrast, no significant relationship between PC1 and discharge was observed in the Mūša or Venta basins.

These results suggest that in the large, hydrologically integrated Nemunas basin, the dominant hydrochemical gradient was partly associated with discharge variability. In contrast, such a relationship was not observed in the smaller basins, where no significant correlation between PC1 and river discharge was detected.

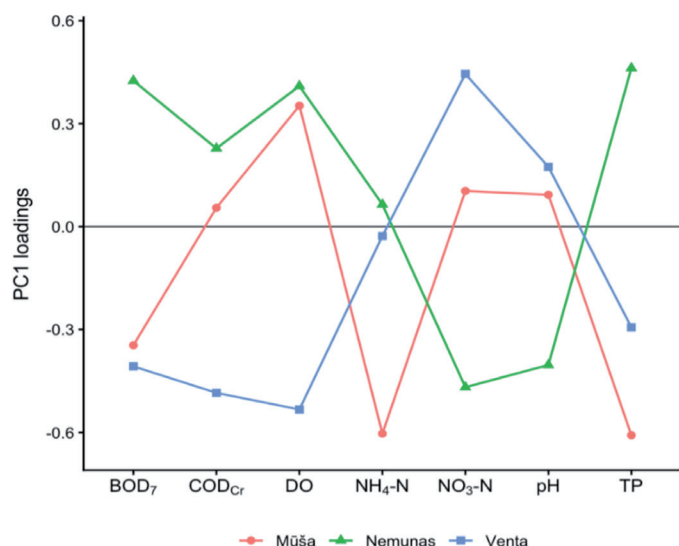


Fig. 5. Loadings of water quality parameters on the first principal component (PC1) in the Nemunas, Mūša, and Venta basins.

Table 4. Pearson correlation between PC1 and WQI across river basins.

Basin	r (Pearson)	p-value	95% Confidence Interval
Nemunas	0.82	< 0.001	[0.70, 0.89]
Mūša	- 0.86	< 0.001	[-0.91, -0.79]
Venta	- 0.40	0.004	[-0.62, -0.14]

Table 5. Spearman correlation between PC1 and discharge (Q).

Basin	ρ (Spearman)	p-value
Nemunas	-0.48	0.001
Mūša	0.01	0.921
Venta	-0.11	0.455

Structural Stability of the WQI–Dominant Gradient Relationship

Bootstrap analysis was performed to evaluate the stability of the relationship between WQI and PC1. In the Nemunas basin, the median absolute correlation was 0.76 (IQR: 0.72-0.79), indicating a relatively stable association across resampling iterations. In the Mūša basin, the median $|r|$ was 0.86 (IQR: 0.75-0.92).

In contrast, the Venta basin showed lower and more variable correlation values (median $|r| = 0.37$; IQR: 0.28-0.49). The distribution of bootstrap-derived correlation coefficients across basins is presented in Fig. 6.

These results indicate that the relationship between WQI and the dominant hydrochemical gradient is more stable and consistent in the Nemunas and Mūša basins, whereas in the Venta basin, this relationship is weaker and more variable across resampling iterations.

Overall, this confirms that WQI sensitivity to the dominant hydrochemical gradient depends on the type

of system organization and spatial scale. A conceptual illustration of the proposed structural relationship is presented in Fig. 7.

Discussion

The results of this study indicate that WQI behaviour varies among river basins with differing hydrological organization. Although an identical calculation procedure was applied across all systems, differences were observed in variability patterns, dominant hydrochemical gradients, and the strength of association between WQI and multivariate structure. This suggests that the interpretation of composite indices may depend on basin-specific structural characteristics.

Mean WQI values alone did not fully reflect differences in internal variability organization. In the Nemunas basin, a larger proportion of total variability was concentrated along the first principal component, whereas in the Mūša and Venta basins, variability was distributed more evenly across multiple components. Although PC1 explained less than half of the total variance, differences in variance concentration among basins indicate contrasting degrees of dimensional organization.

Such patterns are consistent with studies demonstrating scale-dependent relationships between hydrological processes, landscape structure, and water quality dynamics, as well as broader evidence that

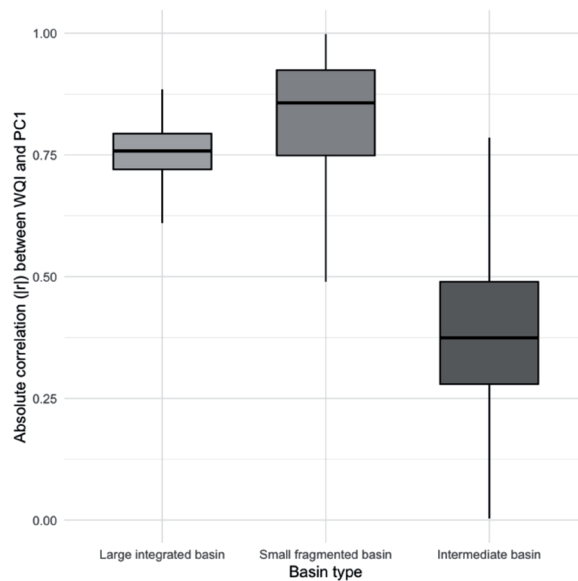


Fig. 6. Bootstrap distribution of absolute correlation ($|r|$) between PC1 scores and WQI across basins of contrasting structural organization.

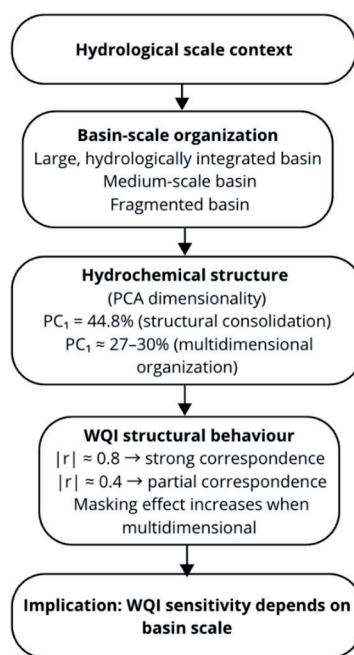


Fig. 7. Conceptual model of scale-dependent structural sensitivity of WQI.

dominant ecological and biogeochemical processes shift across spatial extents [20, 21]. In hydrologically integrated systems, cumulative loading and mixing processes may promote partial homogenization of hydrochemical signals, while smaller or more heterogeneous systems may exhibit stronger localized variability.

The moderate overall correlation between WQI and the dominant principal component indicates that the index captures a substantial portion of the primary hydrochemical gradient, but does not fully represent multidimensional variability. This finding

is consistent with previous research showing that aggregation procedures inevitably reduce multivariate information content [22]. Studies evaluating alternative WQI formulations have demonstrated that parameter selection, weighting schemes, and aggregation rules influence index behaviour [23–27].

Aggregation may also introduce partial masking of secondary gradients, whereby dominant parameters disproportionately influence final index values while multidimensional covariance structures become attenuated. Similar structural sensitivity to seasonal and

hydrological dynamics has been reported in landscape–water quality threshold analyses [28].

Multivariate approaches, including PCA, enable identification of dominant gradients and covariance structures that may remain partially concealed within composite indices [29, 30]. Several studies have explicitly recommended integrating WQI with multivariate diagnostics to enhance interpretative robustness [31]. The present findings reinforce this recommendation, particularly in inter-basin comparisons where hydrological integration and spatial organization differ.

Differences among basins further suggest that WQI performance may vary depending on the degree of hydrological integration and discharge influence. In the Nemunas basin, the dominant hydrochemical gradient was significantly associated with discharge, indicating partial flow-related regulation of variability. In contrast, such associations were not observed in the Mūša and Venta basins, where variability appeared less directly linked to annual discharge dynamics.

These results do not diminish the practical usefulness of WQI. The index remains effective for summarizing overall water quality conditions and supporting regulatory reporting. However, in inter-basin comparisons, interpretation should consider how hydrochemical variability is organized within each system. Complementary multivariate analysis can provide additional context and improve the robustness of interpretation.

Several limitations should be acknowledged. The analysis was based on annual mean values, which reduce short-term variability and event-scale dynamics. WQI results also depend on selected parameters and regulatory thresholds, and alternative weighting schemes or seasonal analyses may yield different structural relationships.

Methodologically, station-year observations were treated as independent data points. Although annual aggregation reduces short-term serial dependence, some degree of spatial clustering and temporal autocorrelation may persist in long-term monitoring data. The hierarchical structure of stations nested within basins was not explicitly modelled. Future studies could apply mixed-effects or hierarchical approaches to further refine structural analysis.

Hydrological influence was evaluated using annual mean discharge, which provides a general indicator of flow conditions but does not capture event-scale processes or flow-normalized concentration dynamics.

Overall, the findings show that composite indicators such as WQI provide valuable but simplified representations of hydrochemical systems. Integrating aggregated indices with multivariate diagnostics can strengthen interpretation and support more informed basin-scale water management. Results reflect patterns observed in the studied systems and should not be generalized without further multi-regional analysis.

Conclusions

This study evaluated the structural relationship between the Water Quality Index (WQI) and dominant hydrochemical gradients in three Lithuanian river basins over a 24-year monitoring period.

The results indicate that WQI sensitivity to dominant gradients differed among basins with contrasting hydrological organization. In systems where variability was more strongly aligned with a primary principal component, WQI showed stronger correspondence with the dominant gradient. In systems where variability was distributed more evenly across multiple dimensions, this correspondence was weaker.

These findings suggest that interpretation of aggregated water quality indicators may depend on basin-specific structural organization rather than on spatial scale alone. While WQI remains an effective tool for summarizing overall water quality status, complementary multivariate analysis can enhance interpretative reliability, particularly in inter-basin comparisons.

The study highlights the importance of considering internal variability structure when applying composite indices in long-term monitoring frameworks.

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AI Usage Disclosure Statement

ChatGPT (OpenAI) was used solely for language editing, translation into English, and improving the clarity and readability of the manuscript. It was not used for data generation, data analysis, interpretation of results, development of the methodology, or formulation of scientific conclusions. All AI-assisted text was reviewed, verified, and edited by the authors, who take full responsibility for the final content of the manuscript.

Conflict of Interest

The authors declare no conflict of interest.

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