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ORIGINAL ARTICLE

Methodology for geoinformation modeling of microelement distribution in surface waters: Case study of the Poltava Region (Ukraine)

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Abstract

The article presents an analysis of current research focused on the use of geoinformation technologies for environmental monitoring. A methodology for geoinformation modeling of microelement distribution in surface waters was developed and tested using the example of the Poltava region. The methodology includes stages of preliminary data processing, interpolation using the Triangulated Irregular Network (TIN) method, and spatial analysis of the obtained results. Based on the modeling outcomes, a cartographic model was created that enabled the identification of areas with elevated barium content. It was established that the area of such zones increased from 4.24% to 37.55% in the period 1991–1993 compared to 1985–1988. A generalized scheme for the environmental assessment of impact on natural components was proposed, which can be adapted to monitoring the condition of water bodies in various regions. The proposed approach can be used to assess anthropogenic pressure, including the impact of military actions, on the quality of surface waters.

Key words: geoinformation modeling, surface waters, TIN method, spatial analysis, environmental monitoring, anthropogenic impact

1 Introduction

1.1 Problem statement

Surface water pollution is one of the most pressing environmental challenges of our time, as the quality of water resources directly affects public health, biodiversity conservation, and the resilience of ecosystem functioning. The accumulation of toxic elements in the environment disrupts ecological balance, leading to the degradation of water bodies and soils, as well as the bioaccumulation of harmful substances in living organisms, including humans. Therefore, monitoring the content of heavy metals in natural environmental components is a critical task that enables the assessment of pollution levels, identification of potential sources of anthropogenic impact, and justification of measures to mitigate ecological risks.

Traditional approaches to assessing the condition of surface waters are mainly based on localized field measurements and offer limited capacity for spatial analysis. Such methods do not reveal regional patterns of pollution distribution and fail to provide timely updates of environmental information across large territories. Moreover, regular field investigations require considerable financial and time resources, which complicates the implementation of systematic monitoring. In this context, the development of methodological approaches that enhance the efficiency of available data processing and reduce dependency on the frequency of sampling – particularly through the use of geoinformation modeling tools – has become increasingly relevant (Parra, 2022; Oztuna, 2023).

Geographic Information Systems (GIS) are considered a powerful tool for integrating, processing, and visualizing spatially distributed environmental data, including information on the content of chemical elements in natural components, particularly in surface waters (Pal et al., 2025; Klymchuk, 2019). The use of GIS technologies enables the application of a wide range of spatial interpolation

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methods, including Inverse Distance Weighting (IDW), kriging, machine learning algorithms, and triangulation-based approaches such as the Triangulated Irregular Network (TIN). These methods support the creation of cartographic models of contaminant concentrations that reflect the spatial structure of pollution and assist in identifying potentially hazardous areas.

Despite the growing integration of GIS in environmental monitoring, several methodological aspects remain insufficiently addressed. These include the adaptation of models to the actual spatial distribution of sampling points, the variability of input data, and the rationale behind selecting interpolation methods (Nisansala, 2022; Jha et al., 2010). The lack of standardized criteria for algorithm selection, the complexity of parameter adjustment based on specific regional characteristics, and the need for comparability of results over long-term monitoring periods present significant challenges to researchers.

Accordingly, the development of adaptive GIS-based modeling techniques becomes especially relevant. These approaches should account for the nature of the input data, morphological features of the territory, and spatial heterogeneity of the study environment. They must ensure a reliable assessment of surface water conditions and be suitable both for rapid environmental analysis and long-term monitoring, including the evaluation of anthropogenic pressures and the consequences of military activities.

1.2 Objective of the study

The objective of this study is to develop a methodology for geoinformation modeling of the distribution of microelements in surface waters and to evaluate the effectiveness of its application for constructing cartographic models that provide spatial interpretation of water sample analysis results. The proposed approach is aimed not only at modeling concentrations within water bodies, but also at assessing the territorial distribution of environmental risks to water resources within the hydrographic system. The methodology is designed to be adaptable to various regional conditions and can serve as a tool for environmental monitoring within systems for evaluating anthropogenic impact.

1.3 Review of recent research and publications

The use of GIS for environmental monitoring of surface waters is an important direction in current research. A significant number of scientific publications are dedicated to analyzing the spatial distribution of pollutants, assessing ecological risks, and forecasting changes in the composition of aquatic ecosystems under the influence of anthropogenic factors (Aydöner, 2024; Maliqi and Penev, 2019).

Special attention in scientific literature is devoted to the development and testing of spatial interpolation methods. The most common among them are kriging, IDW, TIN, as well as machine learning models such as Random Forest, XGBoost, and neural networks. Different authors analyze the advantages and disadvantages of each method depending on data type, sampling point density, and the required level of detail. For example, studies (Shukla et al., 2025; Bilolikar et al., 2023) demonstrate the effectiveness of machine learning for analyzing the chemical composition of water, while (Nisansala, 2022; Jha et al., 2010) present evaluations of different interpolation methods under conditions of complex spatial data structure.

In the context of surface water pollution assessment, one of the methods used in the case of unevenly distributed point data is triangulation (Tamilenthi et al., 2011; Semenchuk, 2022). This method enables the creation of continuous surfaces that preserve local distribution features and is less sensitive to anomalies than some other interpolation approaches.

Nevertheless, despite the abundance of publications on the spatial analysis of pollution data, many of them focus either on local issues or short-term changes in aquatic ecosystems. Insufficient attention is given to the development of unified, adaptive methodological approaches that can be applied to long-term monitoring in different regions while accounting for the specificity of input data.

In view of the above, this study proposes a methodology for geoinformation modeling of microelement distribution in surface waters, based on the use of triangulation as one of the flexible tools of spatial analysis. The methodology is oriented toward practical application in environmental monitoring systems and can be adapted to different sets of input data. This approach enables the generation of detailed spatial models that serve as a basis for further assessment of the ecological condition of water bodies.

2 Main material presentation

One of the key aspects of geoinformation modeling is the use of high-quality input data that ensures the accuracy of the resulting cartographic models. For the testing of the proposed methodology, real historical data were used, obtained during hydro-lithochemical surveys of the Poltava region. These surveys provided a significant volume of information and a high level of detail, making them practically ideal for testing spatial modeling approaches.

The hydro-lithochemical survey data for the periods 1985–1988 and 1991–1993 (Table 1) contain information on the concentrations of microelements in surface waters, obtained through mass sampling.

The first stage of data analysis involved the systematization and visualization of the collected information. In particular, the sampling density was analyzed for each survey period (Figure 1), allowing for an assessment of the spatial uniformity of the dataset. A comparison of the two survey phases made it possible to identify differences in spatial coverage of the sampling points, which could potentially affect the interpolation results.

At this stage of the study, it became possible to perform a preliminary analysis of the spatial distribution patterns of microelements in order to identify zones with elevated concentrations, which may indicate the presence of potential sources of pollution. Identifying such areas is important for the subsequent modeling strategy, as the accuracy of spatial modeling largely depends on the quality and representativeness of the input data.

For testing the developed geoinformation modeling methodology, the microelement Barium (Ba) was selected. This decision was based, firstly, on the high completeness of the dataset – barium concentrations were determined in the vast majority of samples for both survey periods, which ensured sufficient spatial coverage. Secondly, barium is an important toxicological indicator with high sensitivity to technogenic impact, particularly under conditions of intensive anthropogenic pressure, which makes it relevant for use in assessing the state of aquatic ecosystems.

To assess environmental risks, threshold concentrations of barium in water were defined and used as reference values in the spatial analysis. Two regulatory documents were analyzed: DSTU 4808:2007 and DSanPiN 2.2.4–171–10 (Ministerstvo okhorony zdorovia Ukrainy, 2010; Derzhspozhyvstandart Ukrainy, 2007). The upper limit of the range of maximum allowable concentrations (MAC) specified in DSanPiN 2.2.4–171–10, which is based on hygienic standards for drinking water quality accepted in EU countries and by WHO, was adopted as the critical threshold.

Before spatial modeling, statistical processing of the input data was carried out, including the calculation of basic descriptive statistics (mean, median, standard deviation, minimum and maximum values) and the analysis of distribution shape. The results showed that the distribution of barium concentrations is close to lognormal, which corresponds to the typical behavior of geochemical indicators in the natural environment.

One of the key steps of the study was the selection of an ap-

Table 1. Volume of measurements obtained during hydro-lithochemical surveys in the Poltava region

No.	Years	Number of samples collected	Units of measurement	Type of analysis	Chemical elements
1	1985–1988	264	mg/dm^3	Semi-quantitative chemical spectral analysis	Ba, Co, Cr, Cu, Mn, Mo, Ni, Pb, Sr, Ti, V, Zn
2	1991–1993	560	mg/dm^3		

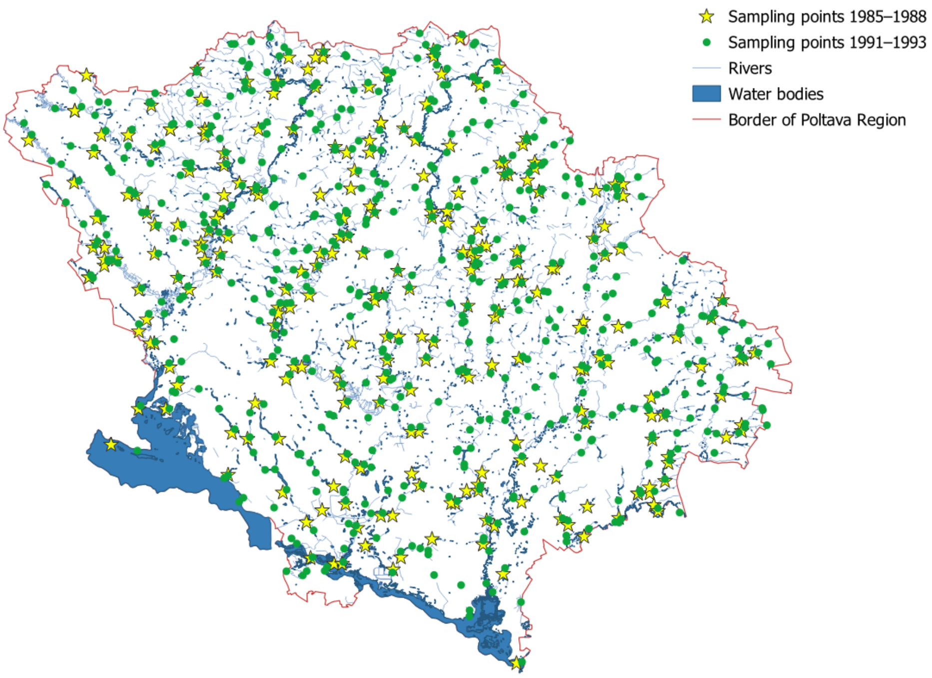

Figure 1. Sampling points from hydro-lithochemical surveys displayed on the map of the Poltava region

propriate interpolation method, as the accuracy of the resulting concentration maps largely depends on the characteristics of the input data. Based on the analysis of previous studies (Nisansala, 2022; Jha et al., 2010; Tamilenthi et al., 2011), the statistical characteristics of the dataset (specifically, the lognormal distribution of barium concentrations), and the research goal – to identify areas exceeding critical thresholds – TIN method was selected. This method provides high sensitivity to local variations and preserves spatial detail, which is important for delineating boundaries of contaminated zones.

Other interpolation methods were excluded for objective reasons. Kriging requires data normalization and variogram modeling, which involves prior logarithmic transformation of values – this was not applied in our case. IDW, although easy to implement, has limited capacity to represent sharp spatial transitions and tends to excessively smooth local features, which complicates the accurate identification of threshold-exceeding zones.

However, the triangulation method also has certain limitations. In particular, it does not perform smoothing of values, which may complicate the construction of predictive models or obscure statistical trends in the data. Additionally, TIN is sensitive to the topology of the mesh: the presence of excessively long triangles may distort local interpretations if the data points are not densely distributed. In cases where the objective is to create a smoothed surface or to detect general spatial tendencies, alternative methods such as kriging or IDW may be more appropriate.

The choice of the optimal approach depends on the distribution of the input data and the objectives of the study, which was taken into account when deciding in favor of the TIN method in this work.

The procedure for constructing spatial distribution maps of microelement concentrations in surface waters involved several key steps: preparation of the input data, interpolation of values using the TIN method, clipping to the boundaries of the study area, and visualization of results in the form of cartographic layers.

At the initial stage, geocoding and systematization of analytical data obtained from the hydro-lithochemical surveys of the two periods (1985–1988 and 1991–1993) were carried out. The microelement concentrations in samples were represented as point objects with spatial coordinates and associated chemical values (in particular, for barium). To ensure the comparability and consistency of the results, all values were standardized to the same unit of measurement (mg/dm^3).

Geoinformation modeling was implemented using the QGIS software, which provides broad capabilities for processing environmental data, performing spatial analysis, and visualizing results. Within this study, the interpolation of microelement concentrations was carried out in QGIS using the TIN method. This method was applied separately to each temporal-spatial slice of the data, allowing for the creation of continuous concentration surfaces. The modeling process considered all available point measurements without prior generalization or transformation in order to preserve local spatial features.

After constructing the TIN models, the resulting layers were clipped using the administrative boundary mask of the Poltava region. This eliminated extrapolation artifacts beyond the actual observation zone and enabled the generation of maps that correspond to the real spatial coverage of the surveys. Additionally, the values were classified according to the levels of exceedance of the critical concentration threshold in accordance with the accepted regulations.

The outcome of these procedures was a set of cartographic models representing the spatial distribution of barium in surface waters, which reflect the pollution dynamics over the analyzed periods (Figure 2). The interpolated data made it possible to clearly identify

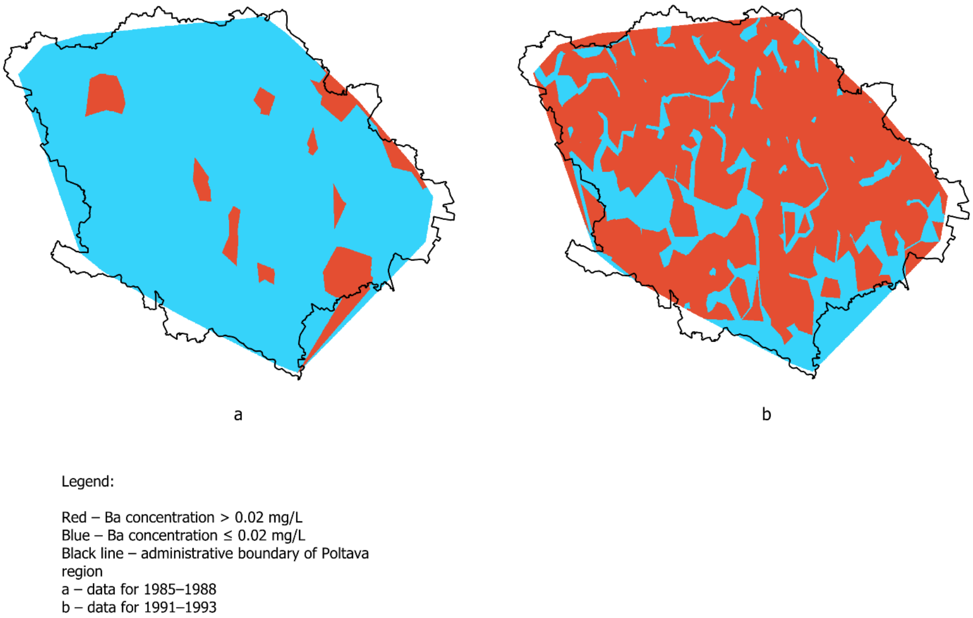

Figure 2. Spatial distribution of barium (Ba) concentration in surface waters of the Poltava region, generated using the TIN method

zones where the concentrations of certain microelements exceed critical thresholds, which is important for environmental risk assessment.

A comparison of the spatial distribution of exceedances across the two temporal datasets revealed not only an increase in absolute values but also a significant expansion in the geographic extent of contaminated areas. While in the first period the exceedances were mostly localized and concentrated in the central part of the region, the second period demonstrates the formation of continuous zones with elevated Ba concentrations that cover most administrative districts. This dynamic may be attributed to anthropogenic activities, a reduction in the natural filtration capacity of watershed systems, or the influence of other exogenous factors.

Based on the interpolated maps of Ba concentrations, binary raster layers were generated in which a value of 1 indicated an exceedance of the threshold level and a value of 0 indicated compliance. Further vectorization of these raster layers resulted in a set of polygons representing exceedance zones, which enabled area-based analysis taking into account the geodetic characteristics of the WGS84 ellipsoid.

The total area of the exceedance zones was calculated as the sum of the polygon areas with a value of 1:

$$S_{exceed} = \sum_{i=1}^{n} A_i, \tag{1}$$

where: A_i – is the area of the *i*-th polygon, and *n* – is the number of polygons representing threshold.

To provide a standardized assessment of the results, the proportion of the exceedance area P_{exceed} relative to the total study area S_{total} was also calculated:

$$P_{exceed} = \frac{S_{exceed}}{S_{total}}. \tag{2}$$

An important step in the implementation of this methodology was the development of Python scripts within the QGIS environment, which enabled the automation of key operations – filtering polygons by value, performing geodetic area calculations, aggregating results, and obtaining indicators in a convenient format. This approach not only improved the accuracy of computations but also ensured the full reproducibility of the analysis for different time intervals and potentially for other regions under study.

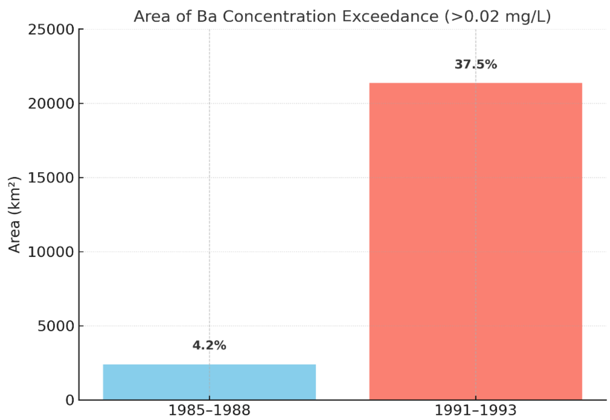

Figure 3. Dynamics of changes in the exceedance area of barium concentration (Ba > 0.02 mg/dm^3) in surface waters of the Poltava region in 1985–1988 and 1991–1993

As a result of the spatial analysis of barium concentrations in surface waters of the Poltava region for the two time periods – 1985–1988 and 1991–1993 – a significant increase was observed in the area where Ba concentrations exceeded the established critical threshold of 0.02 mg/dm^3. According to calculations based on vectorized binary raster layers, in 1985–1988 the area of exceedance was 2,408.62 km^2, which corresponded to 4.24% of the total study area. In the period 1991–1993, the exceedance area increased to 21,354.60 km^2, representing 37.55% of the same territory. The dynamics of this increase are visually presented in Figure 3.

This approach ensured a twofold assessment of pollution:

- geographical – through cartographic visualization of zones where microelement concentrations exceed permissible levels;
- quantitative – by calculating the areas of contaminated territories and their proportion relative to the total study region.

Although the hydro-lithochemical survey data used in this study refer to past decades, they remain a valuable source for testing various geoinformation-based environmental monitoring methodologies. In our case, the volume, spatial coverage, and level of detail of the data allowed for the reconstruction of distribution patterns of microelements in surface waters and for the evaluation of the effectiveness of the applied interpolation and analytical approaches.

It is important to emphasize that the main goal of the study was not to determine the current level of pollution, but to develop a universal methodology suitable for both rapid and long-term monitoring of the ecological status of surface water bodies using up-to-date data. Within this study, the methodology was tested using one chemical element – barium (Ba), which made it possible to verify its applicability in a specific case and lay the foundation for future expansion. The obtained results demonstrate that the proposed approach ensures sufficient accuracy and reliability in identifying zones with elevated microelement concentrations, which is a crucial component in environmental risk assessment.

The proposed methodology can be effectively applied for assessing water quality under current conditions, as it allows for the identification of potentially hazardous areas where the concentrations of chemical elements exceed critical regulatory thresholds. Moreover, it can support the planning and optimization of monitoring systems aimed at the long-term observation of surface water conditions and the forecasting of changes influenced by natural and anthropogenic factors.

Thus, the use of retrospective data has allowed for a clear demonstration of the potential of the GIS-based methodology and its practical value in the context of spatio-temporal analysis of aquatic environments. Although this study focused on the analysis of barium concentrations, the structure of the methodology is universal and can be adapted to other chemical components provided that relevant analytical data are available.

Based on the conducted analysis, a GIS-based scheme for environmental impact assessment was developed, which reflects the logic and sequence of actions as well as the interconnections between the key stages of the research (Figure 4). Although the primary focus in this study was on surface waters, the proposed approach is universal and can be adapted for analyzing other environmental components, including soils and atmospheric air.

The proposed scheme represents a universal approach to spatial analysis of the environmental condition. It integrates the key stages of research – from data collection and processing to modeling, risk assessment, and decision-making. The flexibility of the applied tools allows this methodology to be adapted for analyzing various natural components – surface waters, soils, or atmospheric air. Such an approach is promising in the context of the development of modern environmental monitoring systems and the planning of conservation measures.

Overall, the results of the study confirm the effectiveness of the GIS-based approach as a universal tool for environmental analysis, providing spatial visualization, information systematization, and scientifically grounded decision-making. The presented scheme illustrates an example of a methodology that can be adapted to various regional conditions by modifying only the input data and interpretation approaches. Its application is appropriate both for assessing the current state of the environment and for long-term natural resource management under growing environmental challenges.

3 Conclusions

The proposed methodology for geoinformation modeling of chemical element distribution in surface waters demonstrated its effectiveness in the spatial analysis of the ecological status of water bodies. The testing of this approach using barium as an example confirmed its ability to identify zones with elevated concentrations of pollutants, even under conditions of limited and unevenly distributed sampling. The use of triangulation-based interpolation preserved local spatial features, which positively influenced the accuracy of the cartographic modeling. Subsequent vectorization of binary raster layers enabled the quantitative estimation of areas exceeding the established maximum allowable concentrations, which is crucial for assessing the degree of environmental pressure on aquatic ecosystems.

Despite the retrospective nature of the input data, their volume and level of detail enabled full-scale testing of the methodology, the results of which can be directly adapted to current conditions when up-to-date information is available. The proposed GIS-based model provides a foundation for predictive analysis, which may be implemented through the integration of new datasets, consideration of hydrological, climatic, and other influencing factors, as well as calibration of the model in accordance with environmental changes.

The obtained results have practical value for water resource management authorities and environmental monitoring systems. The methodology can be applied for spatial identification of areas with elevated ecological risk, contributing to more effective monitoring program planning, implementation of preventive measures, and development of ecosystem pressure reduction strategies. Moreover, the results of this study are relevant to the agricultural sector and industrial enterprises, as the quality of surface waters directly affects soil conditions, crop yields, and the safety of production processes.

The universality of the developed methodology allows it to be adapted for the assessment of other environmental components, including soils and atmospheric air, by modifying only the input dataset and analytical parameters. The application of this approach can support the improvement of environmental monitoring systems, enhance the spatial justification of management decisions, and strengthen the scientific basis for the development of environmental strategies in the context of modern challenges, including those caused by military activities.

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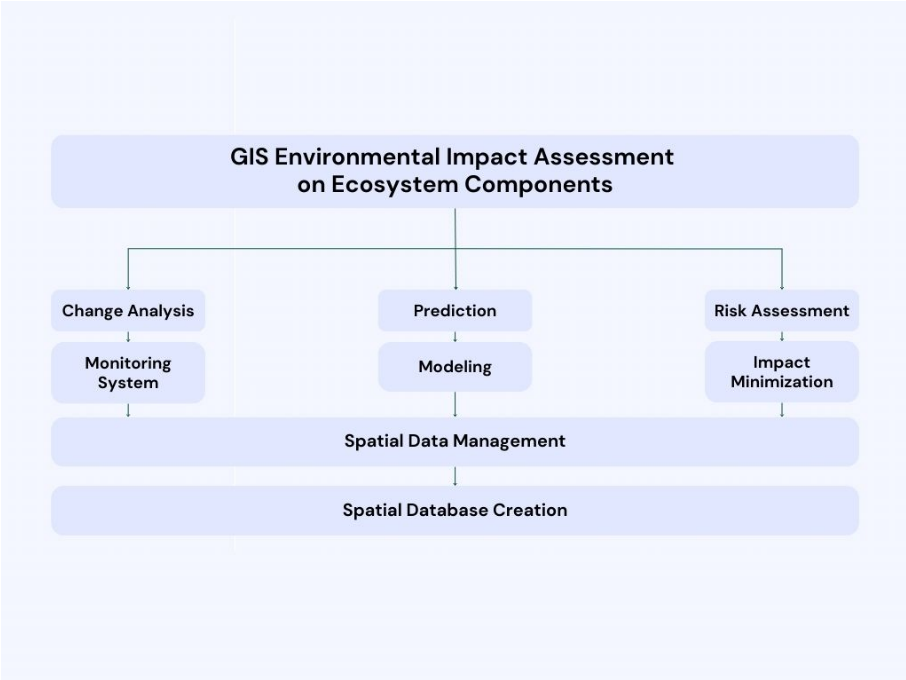

Figure 4. GIS-based scheme for environmental impact assessment on key ecosystem components

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