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Assessment of microelement ecotoxicity in fen for ecological state monitoring

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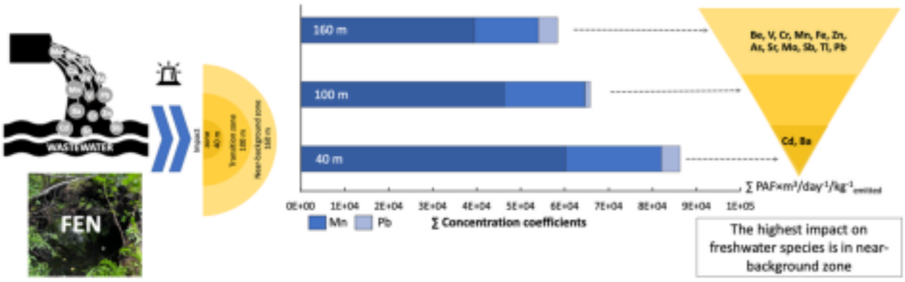
HIGHLIGHTS

- Wastewater discharge contaminating wetland ecosystem 160 m from source of pollution.
- The recommended spatial factor for impact assessment is the size of the water body.
- Freshwater species from conditionally background area have the highest eco-toxicity impact.

GRAPHICAL ABSTRACT



ABSTRACT

Wetlands, including bogs, fens, and swamps, play a crucial role in maintaining ecological balance by absorbing pollutants. They also conserve biodiversity and serve as breeding and migration sites for living organisms whose treated by pollutants entering to the wetland ecosystems. Pollutants entering wetland ecosystems can have detrimental effects on these important functions. The article introduces the method of toxicity assessment of microelements used in the environmental condition monitoring of the Ob River's floodplain fen (Tomsk Oblast, Russia). The impact of freshwater species (PAF m^3day/$kg_{emitted}$) is evaluated by calculating the Life Cycle Assessment Impact score for Be, V, Cr, Mn, Fe, Cu, Zn, As, Sr, Mo, Pb, Cd, Sb, Ba, and Tl at distances of 40, 100, and 160 m from the wastewater discharge site. The study considers the elemental composition and total volume of water from various areas within the research site for assessing freshwater ecotoxicity. 12 out of 15 investigated trace elements have the greatest impact on the freshwater system in the zone of 160 m from the site of anthropogenic impact on the water body. The sampling areas can be ranked based on their $\sum$IS value, with $IS_{160} = 1.3E+11$, followed by $IS_{100} = 7.5E+10$, and $IS_{40} = 1.5E+10$ [PAF m^3day/$kg_{emitted}$].

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1. Introduction

The assessment of environmental toxicity (ecotoxicity) of trace elements in freshwater ecosystems is a pressing issue due to the increasing pollution of water resources (Cui et al., 2022; How et al., 2023). Ecotoxicity, particularly in freshwater systems, serves as an indicator of ecosystem quality (Owsianiak et al., 2023). Environmental toxicity reflects the exposure value resulting from dissolved trace elements in water, taking into account their environmental fate, ecosystem exposure, and the increase in the potentially affected fraction of species. The assessment of trace element impact on ecosystems, based on data analysis, has several uncertainties. These challenges arise from a lack of analytical and ecological-geochemical data (Fantke et al., 2017; Saouter et al., 2017). The data obtained directly by researchers at the test site can help to clarify existing uncertainties (Owsianiak et al., 2023). Proper use of pollution inventory data is critical because it allows prediction of pollution mechanism of the accumulated quantities (Golia and Diakoloukas, 2022), improve the quality of statistical analysis (Morrissey and Ruxton, 2018). The analysis of the inventory database results is also useful for developing an environmental management strategy (Shaheen and Iqbal, 2018).

The goal of the research is to examine the methodology used to assess the ecosystem toxicity of trace elements in wetland ecosystems when incorporating of analytical data in calculations. This approach involves integrating the inventory results with impact assessment modelling.

When modeling the environmental impact of chemicals, it is essential to carefully select data, considering their reliability to minimize the uncertainty of the results. An important indicator of impact is the concentration of trace elements in local environmental media. The distribution of trace elements in environmental media is determined by geological and geographical features, coupled with anthropogenic tension in the area. This distribution subsequently impacts the condition of ecosystems (Bjørn et al. n.d.; Oginah et al., 2023; Yalaltdinova et al., 2018). Various impact indicators are used to measure the impacts of trace elements on ecosystems. For water bodies, these indicators include global warming potential (GWP, in kg CO2-Eq), freshwater ecotoxicity (FETP, in kg 1,4-DCB-Eq, PAF m^3day/$kg_{emitted}$), freshwater eutrophication (FEP, in kg P-Eq), human toxicity potential (HTP, in kg 1, 4-DCB-Eq), marine ecotoxicity potential (METP, in kg 1,4-DCB-Eq), and marine eutrophication potential (MEP, in kg N-Eq) (Verones et al., 2017). The assessment of freshwater ecotoxicity is particularly crucial, given its direct impact on human health (Ersoy et al., 2022; Raudonytė-Svirbutavičienė et al., 2023).

This research highlights the importance of supplementing the pollution inventory database of trace element inputs with the published data (Sharma et al., 2021). To assess the impact of freshwater ecosystems the life-cycle assessment was approached. The Life-Cycle Assessment (LCA) is widely utilized in Europe as a method for monitoring the chemical elements in ecosystems (ISO, 2006a, 2006b; Quevedo-Cascante et al., 2023). Currently, LCA is one of the primary methods in environmental management within the European Union, based on a series of ISO standards (Standards, 1991a; The International Standards Organisation, 2006). The impact of micronutrient pollutants on freshwater wetlands, (with freshwater ecotoxicity as the indicator), is modeled using an adopted Life Cycle Impact Assessment (LCIA) within the framework of LCA procedures. Modeling involves the calculation of the Impact Score (IS), representing the proportion of potentially affected freshwater species. IS allows for the conversion of such environmental media concentrations into masses of contaminants, which can then be translated into a limited number of environmental indicators. The modeling process utilizes the USEtox program, as recommended by the European Commission in their 2013 document « Commission Recommendation of 9 April 2013 on the use of common methods to measure and communicate the life cycle environmental performance of products and organisations Text with EEA relevance» (“Commission Recommendation on the use of common methods to measure and communicate the life cycle environmental performance of products and organisations,” 2013). The USEtox model is suitable for calculating ecosystem impact assessments of non-organic emissions on both global (Karim et al., 2019; Li and Niu, 2021) and country scales (Makarova et al., 2018; Pu et al., 2016; Tarasova et al., 2018). The study includes trace elements, crucial components of metalloenzymes vital for the life activities of organisms. However, these elements can become toxic in excessive concentrations (Bezerra et al., 2019; Bjørn et al. n.d.; Environmental Micropollutants, 2022; Oginah et al., 2023; Oleg G. Savichev et al., 2022; Savichev O.G. et al., 2013; Savichev and Heng, 2021).

The object of the study is the Ob floodplain fen, the area impacted by anthropogenic factors, particularly wastewater discharge. Wetlands (bogs, fens, swamps, etc.) play an important role in maintaining ecological balance adsorbing pollutants. At the same time, wetlands are home to many plant and animal species, including those that may be vulnerable to water toxicity. To conserve genetic resources and biodiversity comprehensive research of freshwater ecological status is necessary (Gibbs, 2000; Pollock et al., 1998; Zhu et al., 2023). Another point is that annual flooding of the floodplain increases the risk of pollution spreading and the infiltration of toxic components into the deep groundwater. Localized at the boundary between the Ob fen and the dry valley, the impact zone experiences multidirectional movements of fen water, both toward the Ob and the watershed. This may cause microelements to flow into different areas of the Ob fen with groundwater (Savichev, 2023). Although potentially toxic trace elements enter all sections of the water body, the differentiation of this data is often overlooked during the assessment of their impact on freshwater ecosystems. This oversight poses a challenge to a comprehensive understanding of the dispersion patterns and potential ecological implications of these trace elements within the aquatic environment. To analyze the accumulation of trace elements in the waters of the Ob fen, a comparative statistical analysis of concentrations in different sites was carried out. Analytical data were then extrapolated into a system for calculating the impact on freshwater species, followed by a comparative analysis.

1.1. Research area

The Ob fen (56°35′12″N 84°10′33″E) is located in the southeast of Western Siberia in the Shegarsky District of Tomsk Oblast. It extends along the left bank of the Ob River basin, forming a strip that ranges from 1.5 to 7 km in width and approximately 100 km in length.

The Shegarsky District (56°33′N 84°04′E) is primarily focused on agriculture and is a major producer of agricultural products in the Tomsk region. According to the 2020 census, the district has a total population of 19 958 people. The administrative center of the district is the village of Melnikovo (56°34′N 84°06′E), which has a population of 8274 people, representing more than one-third of the total population of the district.

The study area is part of the Ob fen, which directly adjoins the village of Melnikovo. The administrative center of the district is Melnikovo village, located 60 km west of the city of Tomsk (56°30′N 84°58′E), with a total population of 8216 inhabitants. The Ob fen is located close to Melnikovo. It is important to note that for several years, the treatment facilities for housing and communal services in Melnikovo have been inoperable. As a result, untreated wastewater is discharged directly into the Ob fen via the sewage collector (*Ob utverzhdenii municipal'noj programmy « Razvitie kommunal'noj infrastruktury municipal'nogo obrazovanija « Shegarskij rajon » na 2021–2023 gody*, 2022). The primary source of pollution in the research profile is wastewater, which begins directly from the wastewater discharge point and runs parallel to the main roads 300–500 m away. Other potential pollutants include petrochemical compounds and heavy metals from local roads.

1.2. *Geology of the research area*

The land relief in the research area is shaped by channel and intravalley accumulation of river sediment and fen accumulation. The surface features a hummock-ridge complex. Erosion scarps are present along the boundary of the dryland area ("Gosudarstvennaja geologicheskaja karta Rossijskoj Federacii masshtaba 1:200 000," 2008).

The geological structure consists of Meso-Cenozoic sedimentary cover and the basement is composed of Paleozoic sediments. The upper part of the section is composed of Neogene-Quaternary formations represented by palustrian and alluvial deposits of the floodplain and floodplain terraces. Below these deposits lie Paleogene sediments, which include sands, siltstones, and clays.

1.3. *The hydrology of the research area*

The section of the Ob River up to its entrance into the Tom River — where the Ob fen is situated —is practically non-flowing; the average annual flow of the studied section of the river is 60 km^3. The annual flow distribution of the Ob River is sufficiently influenced by the floodplain. During the flood season, a significant amount of water dams wide floodplain areas. Then, as the floods recede, most of the water returns to the river bed (Chalov R.S. and Pleskevich E.M., 2001). Annual flooding of the floodplain increases the risk of discharging contaminated fen water into the river system. During periods of low water in summer and autumn there may be an increased impact of fen water on groundwater (Savichev, 2023; Savichev and Heng, 2021), which the local population uses as domestic and drinking water supply.

2. Materials and methods

2.1. *Sampling and research methodology*

The Ob fen water sampling was conducted in June 2022, with the monitoring site located near the village of Melnikovo in the municipal housing and communal services' wastewater outlet (56°32′58.1″N 84°05′36.5″E). Sampling was carried out at distances of 40, 100, and 160 m from the floodplain. The distance of 40 m from the floodplain is considered the zone of influence (impact zone), and the distances of 100 m is transitional zone. The zone at 160 m from the floodplain water composition gravitates to the background area; so, this zone will be referred to as conditionally-background. The wastewater discharged into the Ob fen is classified as sodium hydrocarbonate water, with high levels of ammonium (99 mg/L), phosphate (18 mg/L), chloride (160 mg/L), and sulfate (50 mg/L) (Ivanova et al., 2020).

Surface water samples were obtained at a depth of 0.05–0.10 m from the water surface. For the analysis of microcomponents, the samples were filtered through a syringe membrane filter with a pore diameter of 0.22 μm (composed of nylon) into chemically clean 15 ml Falcon tubes. These water samples were stored in a refrigerator at 4 °C until transportation to the laboratory. At the sampling site, temperature, pH, Eh, and specific conductivity were measured using a portable multimeter HI98194 (HANNA Instruments) and Eh-meter ORP200 (HM Digital).

Concentrations of microelements (Be, V, Cr, Mn, Fe, Cu, Zn, As, Sr, Mo, Pb, Cd, Sb, Ba, Tl) were measured by inductively coupled plasma mass spectrometry using an X-series 2 quadrupole mass spectrometer (Thermo Scientific) in GEOCHI RAS (Moscow).

3. Data processing

3.1. *Statistical data analysis*

Descriptive data analysis, encompassing calculations for minimum and maximum concentrations, median value, and standard deviation, as well as the variation coefficient (VC), was conducted (annex, table 4). Based on the obtained analytical data, it can be assumed that the arithmetical mean and concentration coefficient are sufficient for analyzing the accumulation of chemical elements.

The variation coefficient was used to reflect the extent of the discrete distribution of different element concentrations and to indicate indirectly the activeness of the selected element in the studied environment.

3.2. *Concentration coefficient of microelements*

The concentration coefficient of microelements was calculated in relation to the Maximum Permissible Concentrations (MPC) established for water bodies of commercial fishing importance ("Ob utverzhdenii normativov kachestva vody vodnyh ob'ektov rybohozjajstvennogo znachenija," n.d.) using Formula 1:

$$CC = \frac{C_i}{MPC_i} \tag{1}$$

Formula 1. Calculation of concentration coefficient.

Note: C_i – concentration of chemical i [ppm], MPC – maximum permissible concentrations of chemical i [ppm].

3.3. *Calculation of environmental impact indicator*

To establish a link between the measurement and the model, it is proposed to use a Life Cycle Impact Assessment (LCIA) model. This model is intended to express numerically the environmental impact of the studied elements (Be, V, Cr, Mn, Fe, Cu, Zn, As, Sr, Mo, Pb, Cd, Sb, Ba, Tl) in Ob fen's water.

LCIA is a crucial phase within the Life Cycle Assessment process, based on the ISO standards (Standards, 1991a, 1991b). It is applied to evaluate the influence of microelements such as Be, V, Cr, Mn, Fe, Cu, Zn, As, Sr, Mo, Pb, Cd, Sb, Ba, Tl on the impact category of freshwater ecotoxicity. The research involves modeling the impact of these chemicals on freshwater ecosystems.

The resulting Impact Score (IS) is a LCIA impact score used to characterize damages, expressed as the potentially affected fraction of freshwater species integrated over the exposed volume and time [PAF $m^3day/kg_{emitted}$].

The IS is calculated separately for each chemical using the mass of pollutants released from potential impact sources and characterization factors (CF) for the damage (formula 2) (Fantke et al., 2017). Characterization factors serve as a quantitative representation of the (relative) significance of a specific intervention. For example, the characterization factor for the freshwater ecotoxicity of Cd is 2.1E+06, representing the potentially affected fraction of freshwater species integrated over exposed volume and time [PAF $m^3_{day}/kg_{emitted}$].

The CF of freshwater ecotoxicity is derived from the USEtox model (annex, table 1).

$$IS = \sum Mi \times CFi \tag{2}$$

Formula 2. Impact score calculation.

Note: CF_i – characterization factor of the substance i [PAF*m^3/day/$kg_{emitted}$], $M_{i,x}$ - the total mass of the substance's element i in the environment x [kg].

The total mass of the element in water (M) is calculated according to the formula developed by (F. Bratec et al., 2019; T. Bratec et al., 2019) (formula 3):

$$M = \frac{C_{x,i} \times V_s \times p_s}{10^6} \tag{3}$$

Formula 3. Calculation of the total mass of the element in water.

Note: $C_{x,i}$ is the concentration of emissions in freshwater at each sampling point in ppm. $C_{x,i}$ are derived from our own analytical results; p_s is the bulk density of freshwater, a table value taken from the USEtox documentation [kg/m^3]. V_s is the volume of freshwater for each considered region [m^3].

The volume of water (V_i [m^3]) is calculated by the following formula:

$$V_{w[s]} = A_{[S]} \times fr\_A_{w[S]} \times h_{w[S]} \quad (4)$$

Formula 4. The volume of freshwater calculation (Fantke et al., 2017).

Note: $h_{w\ [S]}$ is a mixed depth of continental freshwater, $fr\_A_{w[S]}$ fraction of freshwater in the continental/global box, $A_{[S]}$ continental system area [m^2].

Values of $h_{w\ [s]}$ and $fr\_A_{w[s]}$ is obtained from the USEtox model database.

The continental system area is calculated as a semicircular square for each section of the fen. The sampling area is composed of three zones with radii of 40 m, 100 m, and 160 m (Fig. 2, formula 1, 3). $A_{[s]}$ is represented as $A_{[S40]}$, $A_{[S100]}$, $A_{[S160]}$.

1) $S_{40} = p \times R^2 / 2$

2) $S_{100} = (p \times R_2^2 / 2)\text{-}(p \times R_1^2 / 2)$

3) $S_{160} = (p \times R_3^2 / 2)\text{-}(p \times R_2^2 / 2)$

Note: S - square for each part of the fen, R – semicircle radius.

Formula 5. Calculation of the semicircular square for each part of the fen.

4. Results

Adequate methodology ensures reproducibility of results (Tokatli et al., 2021).

The analysis of the obtained values is presented in Fig. 3. All values are above the detection limits of the chemical analysis. Notably, the highest concentrations are observed at the wastewater discharge point (40 m).

The calculation of the concentration coefficient indicates an exceedance (10^4n) of the maximum permissible values for all analyzed components except Tl. The anthropogenic nature of the water trace element composition is indicated by previous studies considering wastewater discharge into the fen (Ivanova et al., 2020; O.G. Savichev et al., 2022; Savichev et al., 2022; Savichev O.G. et al., 2013; Savichev and Heng, 2021). There is a significant shift in the content of Be (3-fold), Mo (4-fold), Cd (4-fold), Tl (4-fold), Pb (4-fold), and Cu (9-fold) in the waters of the Ob fen. For 11 out of 15 chemical elements, the difference between the minimum and maximum concentration is within 1.5–2 times.

Results of freshwater ecosystems Impact score calculation is given in Fig. 4.

The chemicals with the highest impact on freshwater species in the impact zone are Sr, Mn, Ba, Zn, Cd, Cu, and V. In the transition area, the chemicals with the highest impact are Sr, Tl, Mn, Zn, Sb, V, Cu, As, Cr, and Fe. In the background area, the chemicals with the highest impact are Sr, Tl, Mn, Zn, Sb, V, As, Cu, Cr, and Fe. The order of chemicals is listed in decreasing order of impact.

In the sampling area located 160 m away from the wastewater discharge source (the region with the lowest concentrations), the analysis reveals the maximum impact score for the majority of considered chemical elements (Be, V, Cr, Mn, Fe, Zn, As, Sr, Mo, Sb, Tl, Pb) (Fig. 4). The exceptions are Cd and Ba. IS calculated for Cu does not change across different sites. Based on the variation in the ecosystem toxicity indicator, the chemical elements can be conditionally divided into two groups. For the first, which includes Be, Zn, Mo, the value ranges from 53 to 63%. The second most numerous group: Be, V, Cr, Cr, Mn, Fe, As, Sr, Tl, Pb varies from 64 to 120%. Within each selected group, certain elements deviate from the typical range of values: Ba (V = 173%), Cd (161%), and Cu (V = 7%).

5. Discussions

5.1. *Microelements' concentration analysis*

Data from the literature indicate that the condition of the fen does not meet established quality standards for natural waters (Ivanova et al., 2020; Savichev et al., 2022; Savichev et al., 2022; Savichev O.G. et al., 2013; Savichev and Heng, 2021).

Water samples collected at a distance of 40 m from the discharge source are characterized as the most polluted compared to the background samples, which is evidently linked to the discharge of wastewater into the fen. The studied area is a floodplain of the Ob River near the dry landfall. Wastewater is discharged from the dry land under the erosion ledge, creating a point source of pollution. Supporting this observation, the sum of concentration coefficients for all trace elements in waters sampled at a distance of 100 m shows a 1.3 times reduction in pollution levels. Mn, Pb, and Cu have the most significant influence on the summation of concentration coefficients (see Table 2 and Fig. 2 in the annex).

According to literature data, the Ob fen is characterized by a high ability to maintain a stable ecological-geochemical state (Savichev et al., 2022).

Changes in the distribution of chemical elements in the Ob fen are evidenced by temporal dynamics. In studies conducted in 2013 (Cu, Pb, Zn), there was a smaller (1.5–5.5 times) difference in concentrations of Cu and Pb between polluted and unpolluted sites, and a larger difference for Zn (5.5 times in 2013 and 2.3 in 2022) (Savichev O.G. et al., 2013). Despite being a point-source pollution, the negative impact spreads to remote areas. Pollution results in increased salinity, macrocomponents, and nitrogen compounds in the water body (Savichev and Kamneva O. A., 2011). There has not been a significant increase in the amount of pollutant components discharged into the waters, since comparing the data obtained with previously published results, the following observations can be made:

1) The concentrations of Cu in the impact zone (40 m) have increased by 1.5 times compared to the levels observed in 2013, while at the remote distances of 100 and 160 m, they have remained consistent with the 2013 levels (0.00n).
2) Zn concentrations at the site of wastewater discharge remain at the level of 2013 (0.0n), and at the distances of 100 m and 160 m from the source of discharge, they are slightly higher than those at unpolluted sites (0.00n).
3) For both the discharge area and the background waters (0.000n), the Pb level is comparable to 2013 values.

Freshwater ecosystems are constantly under pressure from irrigation, domestic, fisheries, and industrial purposes. Improving the accuracy of impact assessments for freshwater ecosystem toxicity is particularly crucial (Tokatli et al., 2021; Tokatlı et al., 2023). The object of the study plays an important role in the formation of the ecological structure of the region (Shemjakina and Simakova T., 2018). The results of the microelement composition of the Ob fen waters provide insights into the state of the freshwater environment. The obtained results expand our knowledge of the fundamental principles of the flow of elements and exchange processes in ecosystems (Tokatli and Ustaoğlu, 2020). When integrated into the LCIA model, this information allows for the identification of potential pollution in the water body.

5.2. *Impact score $_{eco}$ calculation*

The modeling results highlight elements critical to the study. Chemical and toxicological properties of Cd have a negative impact on the ecosystem even at relatively small concentrations in water. The modification of the Impact score eco calculation showed the influence of factors such as the proximity of pollution sources, the concentration of microelements, and the value of their characteristic coefficient on the result. By assessing the data on the accumulation of trace elements in water in conditionally-background, transitional, and impact zones, it was possible to calculate the water volume of each area for further categorization of microelements based on their degree of influence on freshwater species.

12 out of 15 trace elements have the highest impact score in the waters of the conditionally-background area. The influence of the studied area on the impact magnitude of trace elements on freshwater ecosystems was also indicated in other previously published works. An assessment of the Impact score eco for different districts of the Tomsk region showed that the results were influenced by the size of the studied zones.

The impact score indicates that a larger percentage of freshwater species are negatively affected by microelements in the conditionally-background zone than in the impact zone or at the intermediate site.

Cd has the greatest impact on the freshwater ecosystem in the wastewater discharge zone. Cd is a microelement having the maximum characteristic coefficient of freshwater ecotoxicity (annex, Fig. 1). The concentration coefficient of Cd is not maximal among studied elements. The high value of CF suggested by the USEtox model is related to its toxicological and physicochemical properties. Cd poses a high ecological risk and requires urgent attention (Huang et al., 2020; Islam et al., 2017). Therefore, it is recommended to consider the microelement composition of water from areas at different distances from the pollution source to calculate the impact. When estimating the pollution index, it is recommended to consider seasonality (Tokatlı and Varol, 2021). The results of the assessment of the impact of freshwater ecotoxicity can be used to monitor the quality of the ecosystem (Haq et al., 2023; Tokatli and Ustaoğlu, 2020) and extend the inventory database with non-organics.

6. Limitations

1. The study does not aim to conduct an LCA analysis but rather to suggest a modified LCIA method for assessing the impact of microelements on freshwater ecosystems.
2. To examine the dynamics of pollution spreading, we selected three sampling points located at various distances along the profile from the wastewater discharge source. In our analysis, we did not account for permeability anisotropy concerning pollution spreading. Instead, we assumed that the pollution spread radially, based on the findings obtained from the temporal and spatial analysis of the Ob fen's water chemical composition (Kolotygina et al., 2023);
3. The comparison of microelement concentrations was limited to the elements analyzed in the Ob fen based on literature data (Savichev O. G. et al., 2013).
4. The impact on the fraction of potentially affected freshwater species integrated by volume and time of exposure was modeled using the characterization factor table of the USEtox model.
5. The methodology recommended in the USEtox model documentation was used to calculate the volume of freshwater available for converting trace element concentrations to their mass. The calculation did not incorporate pollution spreading fluxes and rates.

7. Conclusions

The publication presents an approach to utilizing analytical data in studies on freshwater ecotoxicity. Chemical analysis has verified the presence of potentially hazardous trace elements in the water of the Ob fen at concentrations that surpass the MPC for water bodies intended for fishery purposes. The introduction of trace elements into the water from the discharge source affects all three zones. The concentration of microelements in the water diminishes as distance from the pollutant source increases (in 1.5 times from 40 to 160 m). The water does not meet fishery standards, even at the farthest sampling point from the wastewater discharge point. The concentrations indicate a high level of potential impact on biota.

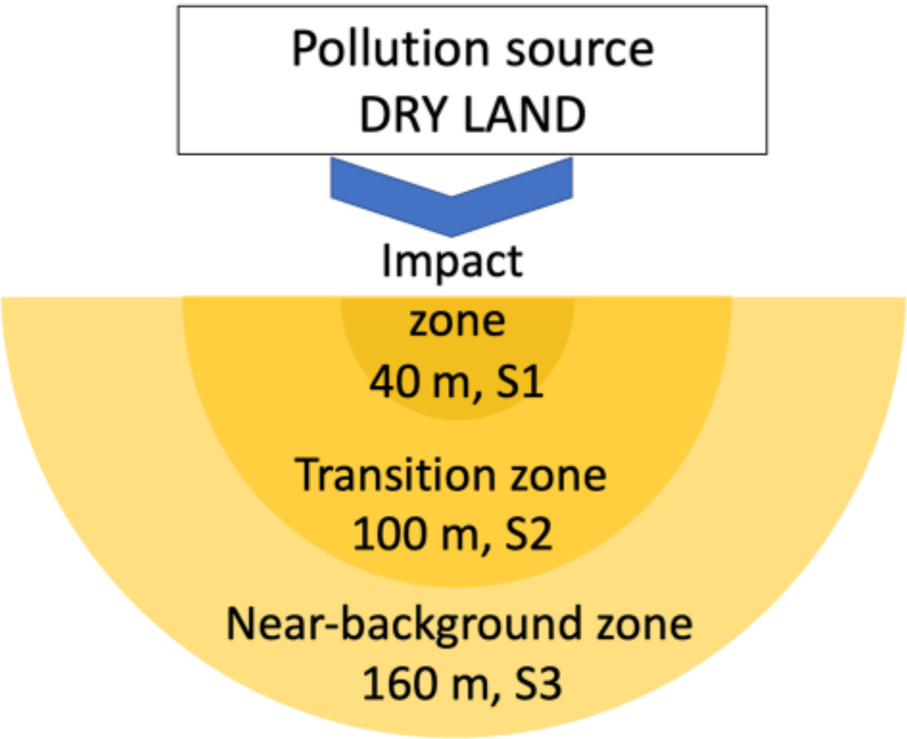

Fig. 1. Fragment of the Ob fen map.

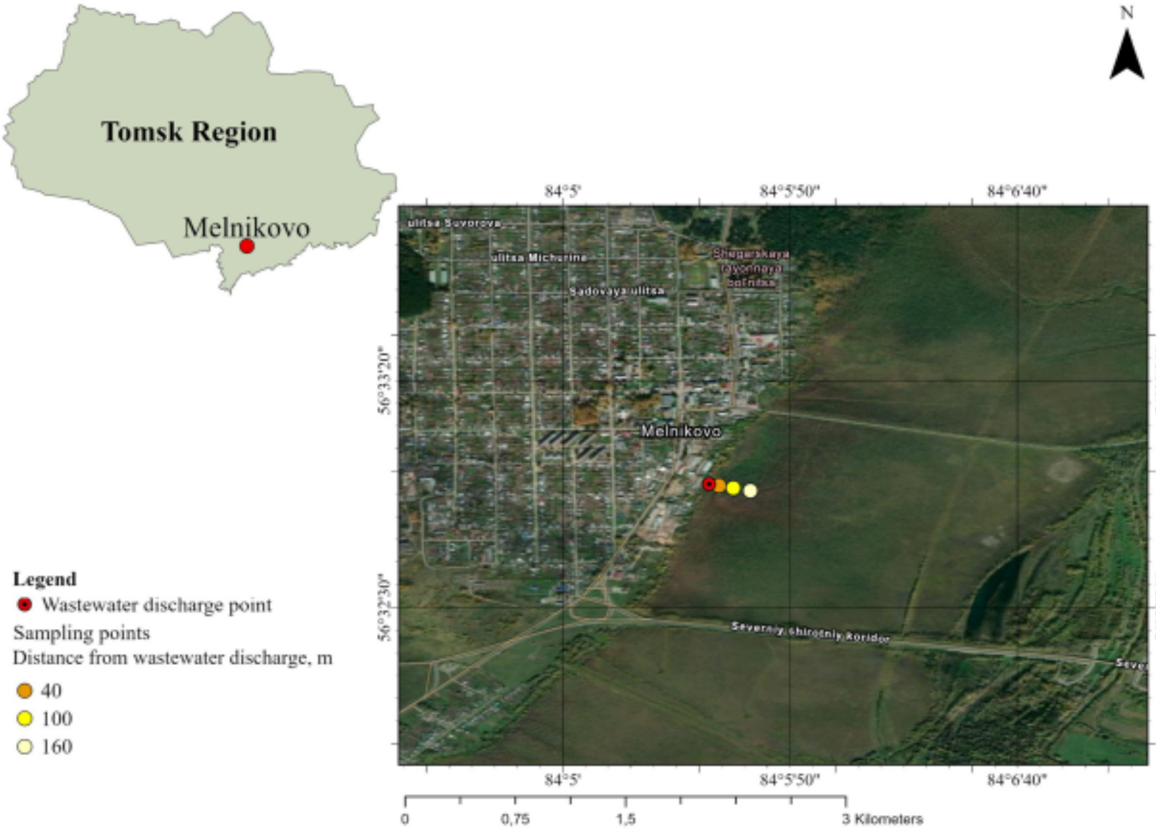

Fig. 2. Sampling points of Ob fen. Note: S1 – Impact zone, S2 – transition area, S3 – background area.

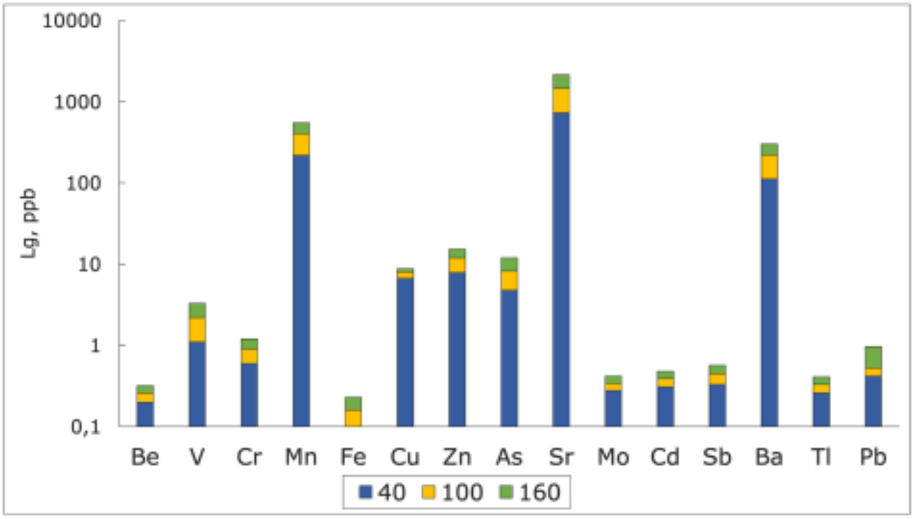

Fig. 3. Chemical composition of Ob fen water, [ppb], Lg scale.

The modeling of the impact on freshwater species, categorized by the proximity to the wastewater discharge source, enables the division of the elements into areas of maximum impact. The greatest impact occurs in the zone farthest from the point of wastewater discharge, despite the minimal concentrations of trace elements compared to the other two areas. This is due to the largest area of this site. The IS_{160} exceed IS_{100} by 2 times and IS_{40} by 9 times. The modeling results emphasize essential factors for the study, such as Cd, whose chemical and toxicological characteristics have a considerably adverse impact on the ecosystem ($CF = 2.1E+06$ [$PAF*m^3/day/kg_{emitted}$]), even in relatively low quantities. Analysis of trace element concentrations allows consideration of incoming pollution flows, and impact modeling translates these results into potential hazard values.

In terms of methodology, modeling the consequences of trace elements on freshwater ecosystems is a potent instrument for informed decision-making in environmental protection and sustainable development.

CRediT authorship contribution statement

A. Belyanovskaya: Conceptualization, Data curation, Methodology, Writing – original draft, Writing – review & editing. **E.A. Soldatova:**

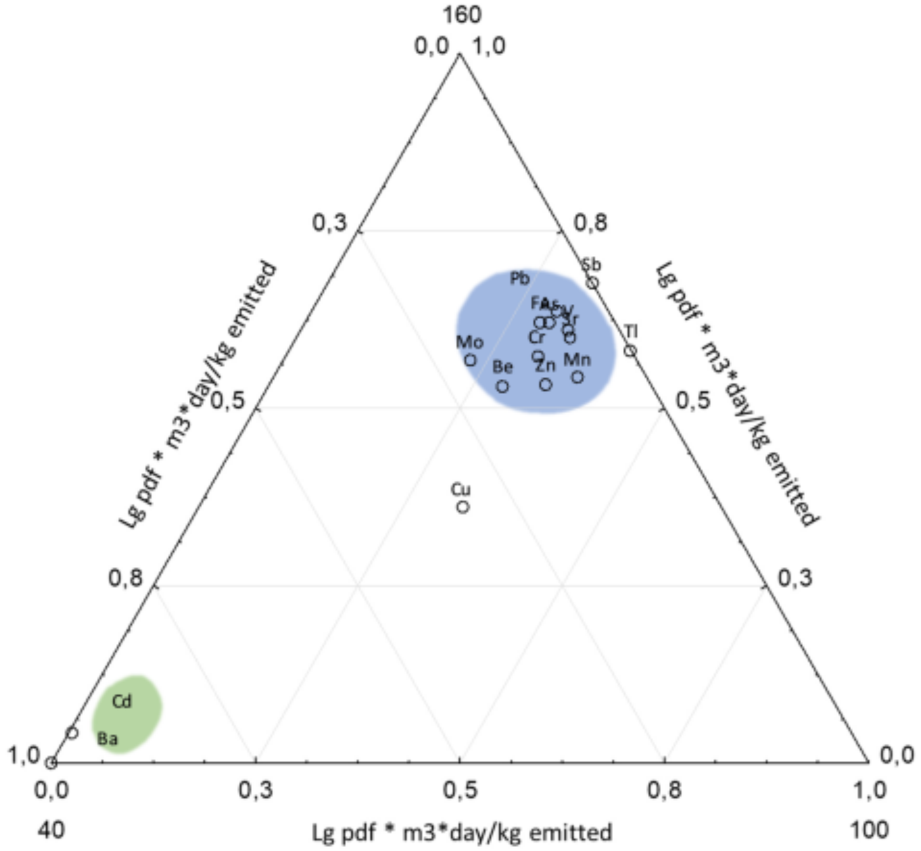

Fig. 4. Freshwater ecosystems Impact score, [PAF*m^3/day/$kg_{emitted}$], Lg scale.

Data curation, Investigation, Methodology, Writing – original draft, Writing – review & editing. **V.N. Kolotygina:** Methodology, Visualization, Writing – original draft. **B. Laratte:** Formal analysis, Supervision. **N.P. Korogod:** Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.chemosphere.2024.141163.

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