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Intelligent visualization and modeling of phytogeochemical profiles of industrial dumps in Donbass

Inteligentna vizuelizacija i modeliranje fitogeohemijskih profila industrijskih deponija u Donbasu

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Abstract: The paper contains information on the features of phytogeochemical profiles for industrial sites in Donbass – coal mine dumps. The studies were conducted using a multi-stage system of using statistical techniques in mathematics and elements of artificial intelligence in making decisions on the selection of priority pollutants and reference chemical elements to restore missing data. Intelligent visualization of analytical control data of biogeochemical processes is a unique profile of information reflecting similar series for the nature of technogenic pollution of the environment. For the first time, gradients of accumulation of individual elements in the tissues of an indicator plant were established, which is considered in the future as a remediant in the restoration of disturbed ecotopes of Donbass.

Keywords: technogenesis, intelligent data visualization, statistical methods, phytogeochemistry, phytoindication, environmental monitoring, Donbass.

Sažetak: Rad sadrži informacije o karakteristikama fitogeohemijskih profila za industrijske lokacije u Donbasu - odlagališta rudnika uglja. Studije su sprovedene korišćenjem višestepenog sistema korišćenja statističkih tehnika u matematici i elemenata veštačke inteligencije u donošenju odluka o izboru prioritetnih zagađivača i referentnih hemijskih elemenata za obnavljanje nedostajućih podataka. Inteligentna vizuelizacija analitičkih kontrolnih podataka biogeohemijskih procesa je jedinstven profil informacija koji odražava slične serije za prirodu tehnogenog zagađenja životne sredine. Po prvi put su utvrđeni gradijenti akumulacije pojedinačnih elemenata u tkivima biljke indikatora, što se u budućnosti smatra remedijantom u restauraciji poremećenih ekotopa Donbasa.

Ključne reči: tehnogeneza, inteligentna vizuelizacija podataka, statističke metode, fitogeohemija, fitoindikacija, monitoring životne sredine, Donbas..

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INTRODUCTION

The system of quantification of natural environment objects under technogenesis conditions involves the use of certain analytical procedures and methods of secondary synthesis if the set of information on the state of a local ecosystem represents large arrays of quantitative results (Ermakov, Jovanovic, 2012; Korniyenko, Kalaev, 2022; Rouhani, Skousen, 2023). For most of the territory of Donbass, the introduction of methods for restoring disturbed ecotopes is a priority environmental task due to significant transformations as a result of increasing anthropogenic activity (Dogadkin et al., 2024; Nespirnyi, Safonov, 2024; Safonov et al., 2024).

The purpose of the work is to visualize a model of several phytogeochemical profiles characteristic of the waste heaps of Donbass using methods of mathematical statistics based on elemental analytical control data. At the same time, an important stage in the advancement of scientific research is the approach of using the capabilities of artificial intelligence for: 1) restoring missing data, 2) reconstructing historical processes of nature management in the region, 3) modeling those patterns that are characteristic of the industrial environment, 4) making decisions about the belonging of a specific sample of the phytogeochemical environment to a specific system of the geochemical province in a technogenically disturbed region.

Previously conducted studies (Safonov et al., 2023, Safonov et al., 2024; Zinicovscaia et al., 2024) obtained some patterns of migration and accumulation of chemical elements (including toxic and man-made) for the Donbass ecosystems under conditions of intensive economic activity.

Professor V.V. Ermakov (1939-2025 years of life) contributed greatly to the development of such research; he is the author of the experimental ideology and the beginning of work on collecting plant materials at man-made sites in the modern conditions of Donbass. The Vernadsky Institute of Geochemistry and Analytical Chemistry greatly helps scientists in Donbass, taking into account the difficult material conditions that arose during the military events.

The task has been completed within the framework of the youth laboratory “Diagnostics and mechanisms of adaptation of natural and anthropogenically transformed ecosystems of Donbass”, Azov-Black Sea Mathematical Center. Part of this work performed at the Vernadsky Institute of Geochemistry and Analytical Chemistry was supported by the Ministry of Science and Higher Education of the Russian Federation, within the budget theme of the Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences.

1. MATERIALS AND METHODS

The work uses analytical control metdods: atomic absorption, mass spectrometry with inductively coupled plasma, and the neutron activation analysis method. The importance of such studies is due to the fact that there is no data on modern pollution in the region, and military events are also underway, which also adversely affects the sustainability of ecosystems. At the same time, it becomes possible to conduct an examination in a partially remote format using a database and artificial intelligence programs to restore a holistic environmental picture in dynamics and modern development.

For cases when the results of analytical control and structural-botanical examination represent fragmentary information, a special method of restoration (imputation) of missing information in a specific series (sequence) of features has been developed.

The presented work functionally combines methodological techniques for assessing the ingredient composition of plants (using the established remediant Phleum pratense L. as an example) as part of the programs for phytochemical assessment of raw materials, and takes into account cenotic patterns using the example of successional processes of vegetation formation under the impact of accumulated damage objects. The main objective of the study was to visualize the data, the correct interpretation of which is possible with a more detailed examination and accumulation of information.

Geophysical and geochemical parameters in industrially developed regions are characterized by a certain dynamism of variability if specific interventions are observed (Jovanović et al., 2023; Kolesnikov et al., 2022; Yeprintsev et al., 2023), which is relevant for the territory of Donbass during military events (Dogadkin at al., 2024; Safonov et al., 2024). Some phytogeochemical features of coal mine dumps in Donetsk and Makeyevka were determined. The results obtained are in the stage of constant supplementation with new information, which determines the need for their ordering. Phytogeochemical series of contrasting conditions of Donbass were formed for different taxa and zones of ectopic confinement, for example, using indicator species of bryophytes (Zinicovscaia et al., 2024). The work uses methods of geochemical control and the possibility of using data for remediation of disturbed soils, ecotopes in an industrially tense region (Fernández-Braña, Salgado, 2023), which is typical for places and areas of mineral extraction,

construction of coal mines, landscape disturbance and high levels of environmental pollution (Kříbek et al., 2028; Massante, 2015; Zheng et al., 2024).

2. RESULTS AND DISCUSSION

The classical approach to the analysis of data on geochemical provinces and migration flows in geosystems is the pair correlation analysis of a set of digital data, which is an array of information and highlights the pattern of joint entry into the environment. Figure 1 shows the results of the general diagram of the ratio of concentrations and the specificity of accumulation of elements in plant tissues of the indicator species, which is the primary link in the food chain and plays the role of a remediant in the formation of a stable striking cover. This approach ensures success in the processes of greening and preventing erosion of the soil horizon.

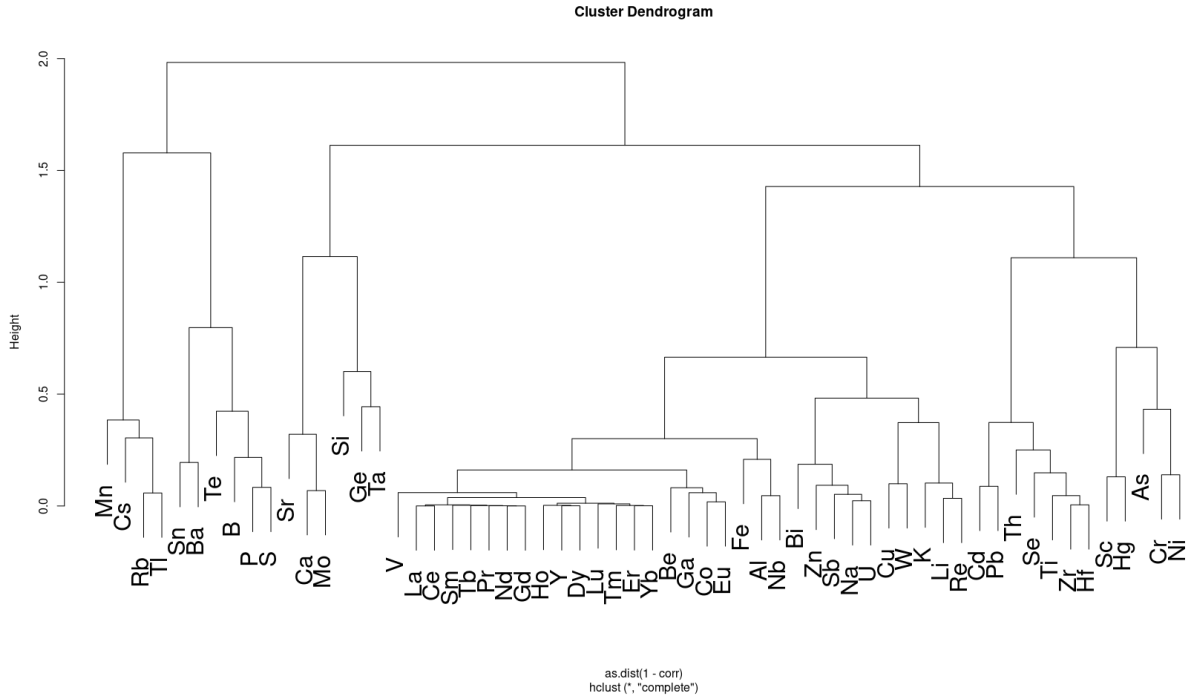

Figure 1. Correlation links between elements in the composition of an indicator plant that forms a stable population during remediation processes in the dumps of coal mines in Donbass

The obtained results confirm that the plant has a high level of accumulation of chemical elements entering the environment precisely with technogenic intervention – during the extraction of minerals and the construction of a waste heap as a place for the accumulation of hazardous waste and requiring optimization of the environment. By means of such analysis, we have established toxic and mobile elements that are of the greatest importance in the migration flows of matter as a result of technogenesis. In general, 2 large groups of elements are separated, antagonizing each other (left and right parts of grouped values, see Figure 1 - dendrogram). Within each group of accompanying elements, there are also groupings of elements that reflect the joint entry into the plant organism. This was proven with the help of the mathematical apparatus used - statistical data on arrays of values for seven waste heaps of Donbass.

The significance of such data proves that technogenic elements are not only in the geological environment (the dead part of nature), but also enter into biogeochemical cycles, which leads to their entry into the cycle of active components of living nature. In response to such pollution, a plant can form various structural modifications and even change its life strategy, for example, to reproduce more by seeds under stress conditions or to form additional shoots in order to survive and occupy more free space to capture territory.

The specificity of studying accumulation in a plant organism is important, since the fate of each pollutant element of technogenic nature can differ significantly: some elements can have high concentrations in the soil horizon or parent rock, but do not pose a danger to biological objects, i.e. are not involved in biogeochemical cycles. Nevertheless, as practice shows, most new geochemical provinces in

a contrasting environment of disturbances, explosions, quarrying or mining have an active characteristic of penetrating into the plant organism and further moving along the food chain, ultimately getting into the human body, which is desirable to prevent.

Figure 2 contains information from a more advanced intellectual approach – using the principal component method to analyze patterns obtained in field studies and using analytical control methods. That is, here (Fig. 2) in the projection of the first two principal components, the entire set of established elements is distributed both in relation to each other and in relation to seven geographic points (test sites) that represent different geochemical sources of environmental pollution as a result of the storage of coal production waste in Donbass.

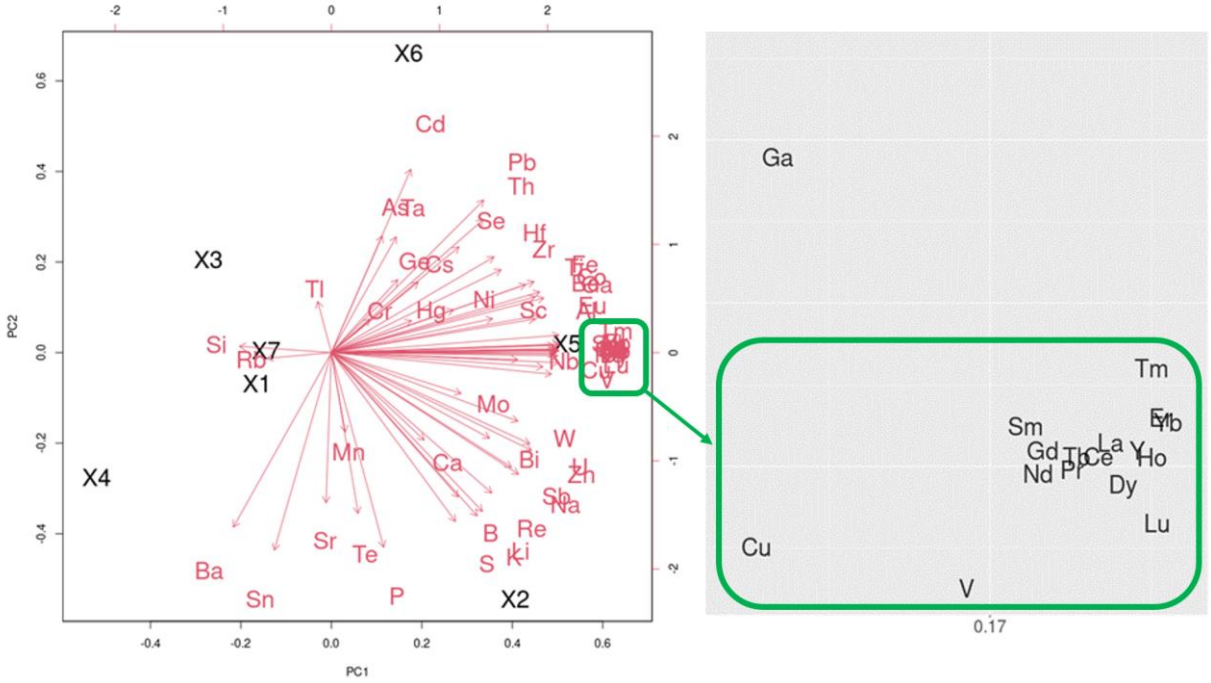

Figure 2. Results of using the principal component method in relation to elements of specific waste heaps in Donbass (decoding of a denser data sector), X1-X7 – localization of waste heaps relative to each other in the projection of the first components

For a more convenient examination of the patterns and results of the analysis, Figure 2 (on the right) contains a detailed diagram of an enlarged section of the primary analysis between the accompanying elements that have a close correlation relationship, which is also proven by the method of paired correlation comparison (Fig. 1) and verified by a secondary intelligent program using the principal components.

Such information has additional characteristics in the analysis of the specificity of pollution and the mechanisms of pollutant entry into the environment. However, the main thing is that the analysis of the principal component method proves the individual geochemical characteristic for the plant collected on individual waste heaps. This allows us to establish a geochemical profile for each waste heap and identify the dominant processes of contamination of harmful substances in the plant organism.

It has been established that the historical processes of the formation of an industrial region are also reflected in the nature of the economic use of the area. Each individual waste heap was built at different times and was created because of mining in a specific layer of underground rock, so it has its own specifics. Since many archival data have been lost because of military actions, scientists of modern research are faced with the task of reconstructing some processes to restore information about the environment. At the same time, only observational methods are not suitable, the system needs to process a large amount of experimental data and methods of intellectual capabilities of calculation systems can solve such a problem.

In the next series of experiments, an attempt was made to specifically develop a program and calculation algorithm for restoring (imputing) missing data that may arise when it is necessary to save

reagents during chemical analysis or when restoring the complete profile of each sample of plant material according to the biogeochemical profile in order to have a complete picture of pollution or compliance with normal living conditions.

From the data set it has been established that for particularly toxic elements their concentrations can be of significant importance in the life of plants even in a small range of variation of their values. Whereas macroelements with a large range of concentrations usually constitute a general background value, ensuring the functioning of the basic physiological needs of the plant, but not radically changing the process of survival in unstable environmental conditions. In most cases, those plant populations were analyzed that have a high adaptation to stress conditions of industrial pollution and military impacts. However, even for such adapted forms of plants, modifications constantly arise that can block the process of development and life of a separate phytocenosis.

We tested the method of an intelligent approach to identifying paired values of conjugate characteristics (Fig. 3). It was necessary to answer the question: are there samples of plant material similar to the seven previously established profiles for waste heaps? Based on the data of the experimental block of industrial botany, it was suggested that the waste heaps of the Kalininsky district of the city of Donetsk and the Krasnogvardeisky district of the city of Makeyevka have a single source of mineral extraction and a common coal seam mined at a depth of 600-800 meters in the 50-70s of the 20th century, can these characteristics of geochemical profiles coincide and how many values are sufficient to reconstruct a geochemical profile based on the absorption capacity of an indicator plant under stressful growing conditions at man-made sites.

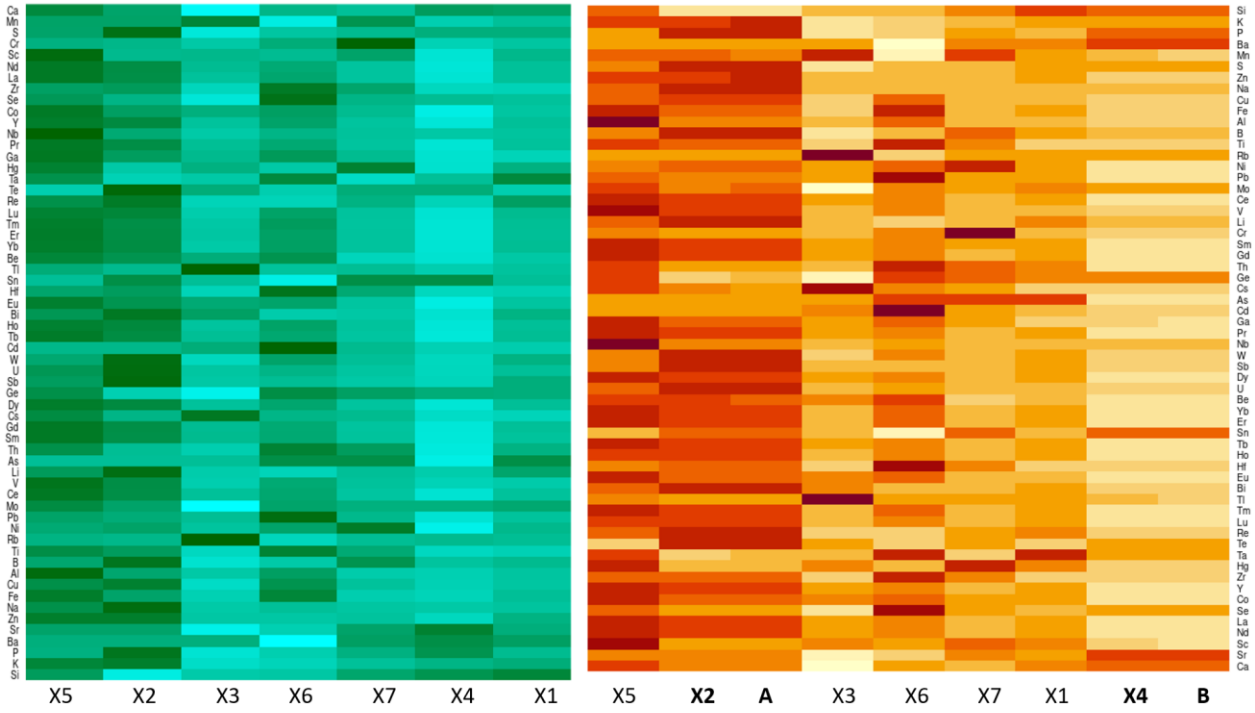

Figure 3. Solution of the problem of determining the associated geochemical profiles in plants using the principal component method and amputation of missing data (as an analogue of the intelligent system for calculating the results of field experiments),
X1-X7 - profiles of the waste heaps of Donetsk and Makeyevka, the profile of waste heap A is characteristic of X2, for waste heap B - X4

In the sequence of conjugated characteristics of individual chemical elements, when new series of the sequence are added (for example, A and B, see Fig. 3), the sequence of the entire series of elements also changes (right part of the figure). However, this does not change the tendency of the mutual relationship between the basic technophilic elements in their interaction and joint entry into the plant organism. Whether such a pattern will be observed for other indicator species must be established experimentally.

The used samples of plant materials of the same species were analyzed for 5, 10, 20, 30, 40 and 50 data available from 60 chemical elements previously

established for seven waste heaps of Donbass. In this case, it is fundamentally important to include in such a list (even with 10 values of their available 60), so that different categories of elements reflecting a large information space within the cluster group are involved in the statistics. That is, with the help of an intelligent system, it was obtained that the minimum sufficient values for reconstructing the entire profile are sufficient if there is information about at least eight chemical elements, provided that each value belongs to a separate cluster group of the most conjugated features established by previously conducted studies in the pair correlation of values. Of course, the number of available samples and analyzed elements increases the accuracy of the experiment.

However, if we are talking about identifying the ecological profile of the territory or the phyto-geochemical profile for the obtained sample in the diagnostics of wildlife, then it is enough to use the values (indices) of contrasting cluster groups.

Examples of such cluster representations can be the following combinations of values (depending on the specifics of the applied methods of analytical control and chemical analysis): 1) Mn-Rb-P-Mo-Ce-Na-Cd-Cr, 2) Cs-S-Ca-La-Fe-Zn-Cu-Ni. For field diagnostics and identification of the kinship of the geochemical profile, such combinations of information on the concentration of the specified elements are complementary in order to conduct an examination, assess the impact on the environment, diagnostics and even use the data in forensics if a sample of plant material is obtained in the area that needs to be established as a result of the investigation. If less than 8 individual concentration values are used, the system does not show the relationship between the profiles and it is not possible to carry out diagnostics and examination in this case.

The 12-component series of data availability on the concentration of elements in a plant (for example, Tl-Ba-P-Mo-Sm-Dy-Eu-Al-Zn-Na-Pb-Hf) provides the possibility of 95-98% accuracy in reconstructing the existing phyto-geochemical profile if the sample was taken under the conditions that were previously studied - from microclimatic features to the specifics of pollution as a result of industrial activity of individual enterprises, for example, metallurgical or metal processing significance.

Therefore, using the capabilities of artificial intelligence application elements, it is possible to optimize the model of geochemical and spatial data visualization and obtain a visual example for full use in the practice of environmental research.

CONCLUSION

Of particular interest is the diagnostics of ecosystems by the specifics of the impact factor of military events, while it has been proven that the concentration of zinc, chromium and lead increases. These three elements are under the close attention of geochemists conducting examinations in places of military disturbances of ecosystems.

In the future, it is important to obtain data not only on the geochemical profile, but also on structural and physiological transformations in plants depending on the specific nature of pollution. The evolutionary biological process allows us to form adaptive mechanisms for the survival of species in contrasting stressful conditions. The accumulated information on plant structures at the present stage undergoes the procedure of quantification and digitalization of data that have qualitative characteristics and recalculated indices in environmental monitoring. For cereal species, data on the microstructures of the periosteal apparatus, terate forms of inflorescences, embryonic modifications during fruit formation, pubescence of leaf parts adjacent to the stem, and the work of the intercalary meristem are promising.

Based on the obtained primary data, a close correlation was found between the elements, which means that a hypothesis can be formulated and further investigated about their joint entry into the plant organism in the following groups: 1) La-Ce-Sm-Tb-Pr-Nd-Gd; 2) Ho-Y-Dy; 3) Lu-Tm-Er-Yb; 4) Co-Eu; 5) Zr-Hf; 6) Rb-Tl; 7) Ca-Mo; 8) Cr-Ni. Technophile elements migrate according to individual scenarios: Mn, Zn, Cu, Cd, Al. Coincidences of the profiles of waste heaps A and X2, B and X4 are noted in addition to the previous descriptions. In new works, cumulative antagonism of pollutants with Ba, Si, Sr and Sn was revealed. In targeted programs for the remediation of damaged systems, it is fundamentally important to operate with the obtained data on the involvement of toxic elements in biogeochemical processes, which allows freely migrating pollutants to be converted into a bound state in the environment.

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