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Creation of natural typing of sections of different thickness of the C_8^H coal seam of the «Dniprovska» mine (Ukraine) according to the germanium content

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(September 19-20, 2022). Brighton, Great Britain





GEOLOGY, MINERALOGY AND SOIL SCIENCE

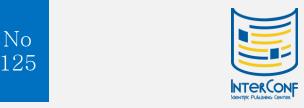
Abstract.

The method of creating an objective (natural) typification of sections of the coal seam of the Dniprovska mine of different capacities according to germanium concentrations has been established and substantiated. The constructed dendrograms of clustering of coal seam areas by Ge content can be used as a basis for developing a natural typification of coal seams for geological and economic evaluation. This will make it possible to make maximum use of already available information and interpret the obtained results in geological and genetic concepts, which provides the possibility of its use for the complex use of mineral raw materials, solving strategic issues of sustainable development of Ukraine.

Keywords:

Germanium
Dendrogram
coal seams
clusters
enrichment zones

(September 19-20, 2022). Brighton, Great Britain



GEOLOGY, MINERALOGY AND SOIL SCIENCE

The relevance of research the content of germanium in coal seams is due to the possibility of its industrial extraction and use as a valuable accompanying component. Currently, coal is the main estimated source of Ge in Ukraine, China, Uzbekistan, as well as in Russia. Ge coal deposits are developed in England, Canada, USA, Ukraine, Russia, etc.

The research carried out is particularly relevant to the decision of the National Security and Defense Council of Ukraine dated July 16, 2021 "On stimulating the search, extraction and enrichment of minerals that are of strategic importance for the sustainable development and defense capability of the state" and Decree of the President of Ukraine No. 306/2021, which introduces this decision is in effect. In these documents, Ge ores are included in the list of strategic importance for the sustainable development and defense capability of the state.

For an objective geological and economic assessment of the possibility of simultaneous extraction of germanium from coal, waste and products of its processing and planning of the most effective organizational and technical measures in this regard, it is first of all necessary to have information about the nature of distribution and the level of concentration of this element in coal. In order to obtain such information, the authors carried out detailed studies of the distribution of germanium over the area and in the cross-section of the coal seam c_8^{H} of the Dniprovska mine field.

Recent achievements. Previously, the peculiarities of the distribution of "small elements" that belong to the group of "toxic and potentially toxic elements" in the coal seams of some mines and geological and industrial areas of Donbas were investigated [1-79]. The methods of natural typification of coal deposits by the content of accompanying elements and oil deposits of the Dnipro-Donetsk Basin by the content of metals were substantiated. At the same time, the analysis of the methods of objective (natural) typification of coal seam areas of different strength according to Ge concentrations in the coal seam has not been performed before.

Purpose of the research. To establish and substantiate the most effective method of creating an objective (natural) typification of sections of the coal seam of the Dniprovska

(September 19-20, 2022). Brighton, Great Britain





GEOLOGY, MINERALOGY AND SOIL SCIENCE

mine of different thickness according to Ge concentrations.

Research methods. The factual basis of the work was the results of 370 Ge analyzes performed after 1981 in the central certified laboratories of production geological exploration organizations of Ukraine from the material of seam samples obtained by production and scientific research enterprises and organizations and measurements of seam thickness. In a number of cases, they were supplemented with analyzes of seam samples taken by the furrow method from duplicate cores and mining operations with the participation of the authors and employees of the geological service of the coal mining production enterprise and geological exploration organizations in the period from 1981 to 2013.

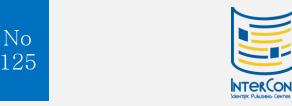
Ge content was determined by quantitative emission spectral analysis. 7% of duplicate samples were sent to internal laboratory control. 10% of duplicate samples were subjected to external laboratory control. The quality of the results of the analyzes (correctness and reproducibility) was evaluated as the significance of the average systematic error, which is tested using the Student's criterion, and the significance of the average random error, which is tested using the Fisher criterion. Since the above-mentioned errors at the significance level of 0.95 are not significant, the quality of the analyzes is recognized as satisfactory.

With the help of Excel 2016 and Statistica 13.3 programs, at the initial stage of processing primary geochemical information, the values of the main descriptive statistical indicators were calculated, frequency histograms of the content were constructed and the distribution law of germanium was established. During the construction of the graphs, all values of Ge concentrations and thickness of the seam were normalized to bring the sample to the same scale regardless of the units of measurement and the scale of the samples.

As is known, the typification procedure is the systematization of objects according to a priori given features. Cluster analysis, taxonomy, pattern recognition, and factor analysis are usually used for this purpose.

It is important that, unlike other methods used in solving typification problems, cluster analysis does not require a priori assumptions about the data set, which does not impose

(September 19-20, 2022). Brighton, Great Britain



GEOLOGY, MINERALOGY AND SOIL SCIENCE

restrictions on the presentation of the studied objects, allows analyzing natural indicators of various types of data (interval data, frequencies, binary data, etc.). The use of cluster analysis for the purpose of typification has a number of advantages, as it allows the division of a large number of studied objects and features into groups or clusters that are homogeneous in the appropriate sense, as well as to reveal the internal structure (at different hierarchical levels) of the sample population. At the same time, like any other method, cluster analysis has certain disadvantages. particular, the composition and number of clusters depends on the selected grouping criteria ("classification strategies"), and the application of different methods corresponding to different conceptual approaches to the selection of taxa to the same samples can lead to significantly different results. Thus, a characteristic feature of cluster analysis, unlike other methods of multivariate statistics, is the strong dependence of the obtained results on the a priori assumptions of the researcher at the substantive level. In our case, a priori assumptions include: lack of hypotheses regarding the number of clusters, their structure on forms; achieving maximum visualization of the breakdown of coal seam sections of different capacity by classes at different scale levels; establishment of a clustering method (algorithm) for the most stable division of the entire set of samples consideration.

In the cluster analysis, it is considered that: a) the selected characteristics allow, in principle, the desired division into clusters; b) units of measurement (scale) are chosen correctly. Thus, the choice of scale in classification procedures plays a significant role. To bring the raw data to the same scale, we normalize it, which is what we did.

To achieve the goal set in the work, in the process of research, clustering was carried out using various methods, which are implemented in the most popular professional statistical software platforms "STATISTICA" and "SPSS"; their analysis was performed and the choice of the most optimal of them was substantiated.

Excel 2016, Statistica 13.3 and IBM SPSS Statistics 22 versions were used in the work.

(September 19-20, 2022). Brighton, Great Britain



GEOLOGY, MINERALOGY AND SOIL SCIENCE

Research and Discussion. In order to develop a methodology for choosing the most effective method of creating an objective (natural) typification of coal seam sections of different strength according to Ge concentrations, the general sample, taking into account the number of samples, was divided into 10 private samples, the main characteristics of which are shown in Table 1.

To perform cluster analysis in the professional software platforms "STATISTICA" and "SPSS" a family of hierarchical agglomerative methods, two-input unification and iterative divisive method of averages is proposed.

Table 1
Main characteristics of private samples of Ge contents

Main characteristics of private samples of Ge contents										
Private samples	1	2	3	4	5	6	7	8	9	10
thickness interval, m	< 0,45	0,45 - 0,50	0,50 - 0,55	0,55 - 0,60	0,60 - 0,65	0,65 - 0,70	0,70 - 0,75	0,75 - 0,80	0,80 - 0,85	> 0,85
Number of samples	35	40	35	19	26	44	58	47	27	22
Normalized median values of Ge content	0,73	0,60	0,48	0,44	0,34	0,28	0,22	0,18	0,1	0,12

The two-input unification method is relatively rarely used for simultaneous clustering of both observations and variables. In this case, it is expected that both observations and variables simultaneously contribute to the detection of clusters, which are further interpreted in geological terms. The main imperfection of the method are problems with the conceptual interpretation of the results, which are a consequence of the fact that the distance between different clusters can be determined by differences in variables. The problematic nature of the conceptual interpretation of the results of the analysis does not allow for its use as an optimal method of solving the task of typing.

The use of the iterative divisive method of K-means for the optimal typification of sites by Ge content also has

(September 19-20, 2022). Brighton, Great Britain





GEOLOGY, MINERALOGY AND SOIL SCIENCE

significant imperfections. It is characterized by the problem of suboptimal solutions inherent in all iterative divisive methods, which consist in sometimes unsuccessful initial divisions of sample populations. Its use implies the existence of a priori hypotheses regarding the number of clusters, and the result of clustering, presented in the form of a system of tables, does not allow to clearly and unambiguously identify and visualize the typification structure. The indicated shortcomings of the method do not allow it to be considered as optimal for the typing of seam sections by Ge content.

The family of hierarchical unifying methods implemented in the used programs refers to the most frequently used methods of cluster analysis. All of them consist of a sequential combination of the most similar objects, which can be visualized in the form of a tree diagram - a dendrogram (which graphically displays the hierarchical structure of the object similarity matrix). This clarity of clustering results is a significant advantage of these methods. As a rule, the objects that are clustered are indicated horizontally in the dendrogram, and the value of the interclass distances at which they are combined (merging coefficient or the merging distance) is indicated vertically. At the same time, as a result of the analysis, non-overlapping groups of clusters are formed, and each cluster is an element of a wider cluster at a higher level of similarity. According to the method of grouping, all hierarchical agglomerative methods in the used programs are divided into the following: the method of single connection ("nearest neighbor"); full connection method ("farthest neighbor"); varieties of the "average link" method - the unweighted "average link" method ("unweighted pairwise average") and the weighted "average link" method; weighted centroid method and Ward's method. In addition, interclass distances can be used in all of the above methods - Euclidean distance (or its square), Manhattan distance ("distance of city blocks"), Chebyshev and Minkovskyi metrics, linear correlation coefficient. With regard to the features of the solved grouping problem, the most optimal is the use of the Euclidean distance as a measure of similarity.

Let us consider in more detail the possibilities of using

(September 19-20, 2022). Brighton, Great Britain

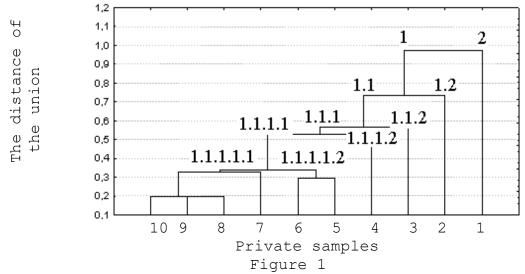


GEOLOGY, MINERALOGY AND SOIL SCIENCE

hierarchical agglomerative clustering methods for the construction of typification of seam sections by Ge content.

The single connection method forms clusters based on the principle of having at least one connection between objects. As a result of the operation of this method, clusters appear as long "chains" "linked together" only by individual elements that happened to be closer than others to each other. Despite the fact that its results are invariant to monotonic transformations of the similarity matrix and the use of the method does not limit the presence of "coincidence" in the data, its practical application for the purpose of typing causes certain difficulties.

On the example of the results of the clustering of deposits by Ge content (Fig. 1), it can be seen that the entire set of deposits, as it approaches the end of the clustering process, forms clusters 1 and 2, which in turn consist of the correspondingly nested subclusters 1.1, 1.2, 1.1.1, 1.1 .2, etc. Analysis of fig. 1 does not allow to determine the number and structure of clusters contained in the source data, and it also significantly complicates the establishment of the number and structure of clusters at other scale levels.



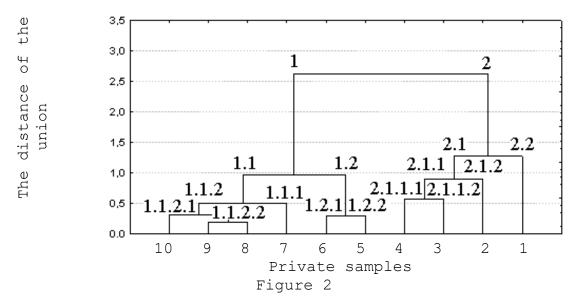
Dendrogram of the results of clustering by the method of single connection of areas by Ge content. Legend: 1, 2, 1.1, 1.2, 1.1.1, 1.1.2, 1.1.1.1, 1.1.1.1.2 - clusters



(September 19-20, 2022). Brighton, Great Britain

GEOLOGY, MINERALOGY AND SOIL SCIENCE

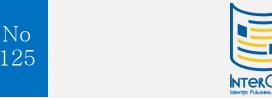
The full connection method (Fig. 2), unlike the method discussed above, imposes stricter requirements for combining objects into one cluster. In this case, there is a tendency to detect relatively compact hyperspherical (in multidimensional space) clusters combining similar objects. Here, the distances between clusters are determined by the largest distance between any two objects in different clusters (ie, the most distant neighbors).



Dendrogram of the results of clustering by the method of complete connection of areas by Ge content. Legend: 1, 2, 1.1, 1.2, 1.1.1, 1.1.2, 1.1.2.1, 1.1.2.2, 1.2.1., 1.2.2, 2.1, 2.2, 2.1.1, 2.1.2, 2.1.1.2, 2.1.1.1 - clusters

Comparison of Fig. 1 from Fig. 2 allows us to reveal a number of advantages of clustering using the method of complete connections. At the same time, if the dendrogram obtained during clustering by the method of single linkage quite convincingly indicates the number and structure of clusters (Fig. 1), then when clustering by the method of complete linkages, there is some change in the areas between clusters and in general, when comparing the results of both methods of identifying the final structure and number of deposits in clusters (Fig. 1, Fig. 2) are not so obvious. In addition, in both cases, the use of only the dendrogram

(September 19-20, 2022). Brighton, Great Britain



GEOLOGY, MINERALOGY AND SOIL SCIENCE

without the involvement of primary data makes it difficult to assign individual objects to one or another cluster, and the structure of the clusters itself is rather poorly revealed.

The "average connection" method was developed by Sokel and Minchener in 1958 as a compromise between the single and full connection methods. In version STATISTICA 13.3 and IBM Statistics 22, two varieties of the method are implemented: the unweighted "linkage average" method ("unweighted pairwise average") and the weighted "linkage average" method. In the first variant of the method, the distance between two clusters is calculated as the average distance between all pairs of objects in them, and in the second, in addition, the size of the clusters (ie, the number of objects contained in them) is used as a weighting factor. Using the number of objects contained in a cluster as a weighting factor assumes "good quality" of the analysis in the presence of clusters of unequal size in the sample. The results of the clustering of reservoir sections by Ge content by both methods in the form of dendrograms are shown in Fig. 3 and fig. 4. The analysis of the given dendrograms allows us to come to the conclusion that in the case of the division of reservoir sections by Ge content, the results of the cluster analysis, respectively, by the methods of unweighted average connection and weighted average connection, in our case, completely coincide.

The weighted centroid method uses the distance between their centers of gravity as the distance between clusters (objects). In fig. 5 shows a dendrogram of the results of clustering by the weighted centroid median method of reservoir sections by Ge content. The analysis of this dendrogram, in contrast to the ones presented earlier (Fig. 1, Fig. 2, Fig. 3 and Fig. 4), allows not only to achieve the most stable division of the entire set of areas under consideration, but also to maximize the visualization of the division of objects by classes into at different scale levels in the absence of a priori hypotheses regarding the number of clusters and their shape.

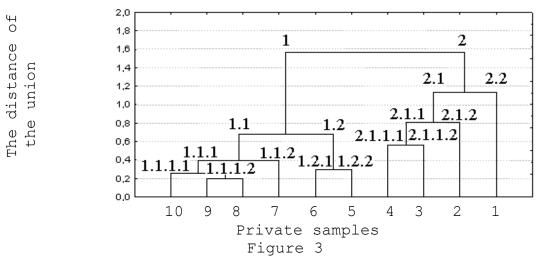
At the same time, the presence and structure of clusters is clearly distinguished, regardless of the large-scale level of their formation, the sequence of unification of individual deposits and their groups into the resulting cluster is clearly traced.

(September 19-20, 2022). Brighton, Great Britain

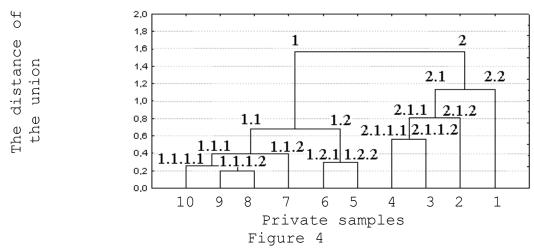


GEOLOGY, MINERALOGY AND SOIL SCIENCE

The presence of these advantages in this case makes it possible to make maximum use of already existing information for the development of natural typifications of areas of coal seams according to Ge content and to interpret the obtained results in geological terms.



Dendrogram of the results of clustering by the method of unweighted average connection of plots by Ge content. Legend: 1, 2, 1.1, 1.2, 1.1.1, 1.1.2, 1.2.1., 1.2.2, 2.1, 2.2, 2.1.1, 2.1.2, 2.1.1.2, 2.1.1.2, 2.1.1.1 - clusters

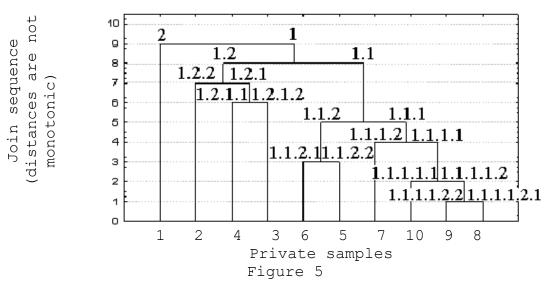


Dendrogram of the results of clustering by the method of weighted average connection of plots by Ge content. Legend: 1, 2, 1.1, 1.2, 1.1.1, 1.1.1.2, 1.2.1, 1.2.2, 2.1, 2.2, 2.1.1, 2.1.2, 2.1.1.2, 2.1.1.2, 2.1.1.1 - clusters

(September 19-20, 2022). Brighton, Great Britain



GEOLOGY, MINERALOGY AND SOIL SCIENCE



Dendrogram of the results of clustering by weighted centroid median method of plots by Ge content. Legend: 1, 2, 1.1, 1.2, 1.1.1, 1.1.2, 1.1.1.2, 1.2.1, 1.2.2, 1.2.1.1, 1.1.2.1, 1.1.2.2, 1.1.1.1.1, 1.1.1.2.2, 1.1.1.1.2.1, 1.1.1.2.2 - clusters

Conclusion. As a result of the conducted research, it was established that the use of the weighted centroid median method of cluster analysis, which is implemented in the professional statistical software platforms "STATISTICA" and "SPSS", is the most optimal for the subjectivity-free researcher of the division of coal seam sections by Ge content into the appropriate taxa.

The constructed dendrograms of clustering of coal seam areas by Ge content can be used as a basis for developing a natural typification of coal seams for geological and economic evaluation. This will make it possible to make maximum use of already available information and interpret the obtained results in geological and genetic concepts, which provides the possibility of its use for the complex use of mineral raw materials, solving strategic issues of sustainable development of Ukraine.

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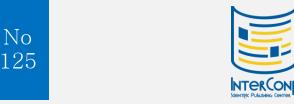
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