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Satbayev University

ХАБАРЛАРЫ

ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК
РЕСПУБЛИКИ КАЗАХСТАН
Satbayev University

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Қазақстан Республикасы Ұлттық ғылым академиясы «ҚР ҰҒА Хабарлары. Геология және техникалық ғылымдар сериясы» ғылыми журналының Web of Science-тің жаңаланған нұсқасы Emerging Sources Citation Index-те индекстелуге қабылданғанын хабарлайды. Бұл индекстелу барысында Clarivate Analytics компаниясы журналды одан әрі the Science Citation Index Expanded, the Social Sciences Citation Index және the Arts & Humanities Citation Index-ке қабылдау мәселесін қарастыруда. Webof Science зерттеушілер, авторлар, баспашылар мен мекемелерге контент тереңдігі мен сапасын ұсынады. ҚР ҰҒА Хабарлары. Геология және техникалық ғылымдар сериясы Emerging Sources Citation Index-ке енуі біздің қоғамдастық үшін ең өзекті және беделді геология және техникалық ғылымдар бойынша контентке адалдығымызды білдіреді.

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MODULE OF THE GEOINFORMATION SYSTEM FOR ANALYSIS OF GEOCHEMICAL FIELDS BASED ON MATHEMATICAL MODELING AND DIGITAL PREDICTION METHODS

Abstract: This paper describes the software module of the geographic information system, developed in the framework of research on methods for intelligent detection of anomalies for deep exploration of deposits. The module is based on the use of a mathematical model for determining the distribution field of a chemical element at a given depth given by the Fredholm integral equation with a Poisson kernel. The software module contains the implementation of algorithms for solving the indicated inverse problem for predictive calculations of the concentration of chemical elements based on measurement data on the day surface, as well as a number of auxiliary capabilities. The algorithm is implemented using the M. Lavrentiev regularization method and the Landweber iteration method. The results of predictive calculations are displayed on the map of the QGIS geoinformation system. The paper describes the structure of the software module and the process of its development, as well as the algorithm of QGIS user actions for interacting with the functions of the module. Implemented module is able to import the initial data obtained as a result of field and laboratory research into the databaseautomatically. The geographic information system database contains data on 29 chemical elements at 3920 points of material sampling in the Novo-Khairuzovsky area of southern Altai, located on the territory of Kazakhstan. The approbation of the mathematical model was carried out by comparing the calculated data with empirical data for gold. On the basis of the comparative analysis, it was concluded that the mathematical model makes it possible to recover the distribution field of chemical elements at a given depth of occurrence with an acceptable accuracy.

Key words: Geoinformatics, geographic information system, geographic information system module, exploration geochemistry, mathematical model.

Introduction. Geochemical searches for mineral deposits are based on the detection of abnormal concentrations of chemical elements or their compounds in rocks, loose sediments, soils, plants, waters and the surface atmosphere.

The most important tool in the geochemical search for minerals is geochemical mapping. As a result of geochemical mapping, maps and graphs of the contents of mineral indicator elements are compiled, for which the interpretation of the identified geochemical anomalies is carried outtaking into account geological and other data; as a rule, only a few of them correspond to industrial deposits. Therefore, the assessment of geochemical anomalies requires a thorough analysis of the scattering conditions and the concentration of chemical elements based on the theoretical laws of geochemistry.

There are a large number of different methods and techniques for developing geoinformation systems (GIS) and their modules. In the work of Yu. I. Shokin, V. P. Potapov [1], a brief analysis of the current state of geoinformation systems is given and promising directions of their development based on modern information technologies (cloud and intelligent systems, big data processing methods) are considered, examples of specific implementations are given in relation to solving problems of mining regions. The pace of development and development of geoinformation systems and technologies can be traced in [2-11].

In the work of R.G. Zuo, E.J.M. Carranza, J. Wang [12], geoinformatics is applied in geological exploration geochemistry for spatial analysis and data visualization. It provides advantages in the study of geochemical patterns and the identification of geochemical anomalies. In the work of M. Yousefi, O.P. Kreuzer, V. Nykanen, J.M.A. Hronsky [13], the careful transfer of conceptual ore deposits into effective maps aimed at exploration is considered and an exploration information system (ISR) is proposed. The purpose of the ISR is exploration, which displays the components of the target mineral system by automatically converting and combining them into a set of weighted factual data (proxy maps), as a result, a map of the prospects of minerals is created. In the study of T. Sun, F. Chen, L.X. Zhong, W.M. Liu, Y. Wang [14], machine learning methods such as the support vector machine, artificial neural networks and the random forest method were used to map the prospects of minerals based on GIS. A comparative analysis of these methods showed that the random forest method surpassed the other two models, achieving greater consistency with respect to changes in model parameters and better prediction accuracy. The article by Y.H. Xiong, R.G. Zuo [15] trains an autoencoder network for encoding and reconstructing a population of geochemical samples with unknown complex multidimensional probability distributions. During training, small probability samples make a negligible contribution to the autoencoder network. These samples can be recognized by the trained model as abnormal samples due to their relatively higher recovered errors.

In the proposed paper, a mathematical model based on the Fredholm equation of the first kind is considered. Due to its ill-posedness, the equation is solved by the Lavrentiev regularization method with the Landweber iterative method. The algorithm was implemented in the high-performance programming language for mathematical calculations Julia.A software module for the QGIS geoinformation system has been developed.

Description of the mathematical model and its numerical implementation. The developed software module is based on the following mathematical model for determining the distribution field of a chemical element at a depth , in which the source of the anomaly is estimated by a flat model, the Fredholm integral equation with the Poisson kernel [16]:

$$A(z) = \int_a^b K(x,y,s)z(y,s)ds = u(x,y), \quad y_{min} \le y \le y_{max}, \tag{1}$$

$$z(y,a) = z(y,b) = 0, \quad z(c,x) = z(d,x) = 0, \tag{2}$$

where u(x,y) is the known field on the day surface, z(y,s) is the sought field at level h below the surface of the earth, $a = x_{min}$, $b = x_{max}$, $c = y_{min}$, $d = y_{max}$,

$$K(x,y,s) = \frac{h}{\pi(x-s)^2+h^2}. \tag{3}$$

Problem (1)-(3) belongs to the class of inverse problems and is ill-posed.

Due to the complexity of obtaining an analytical solution to the problem (1)-(3), a numerical method is used for its solution in this work. Let us dwell in more detail on the question of the numerical implementation of the integral equation (1). Define a rectangular domain Ω that covers the set of sampling points on the day surface. In the resulting domain Ω, we introduce a homogeneous difference grid $\omega = \{(x_i, y_j),\ x_i = x_{min} + i\Delta s,\ y_j = y_{min} + j\Delta y,\ i = \overline{1,n},\ j = \overline{1,m},\ x_n = x_{max},\ y_m = y_{max}\}$, where $\Delta s = (x_{max} - x_{min})/n$. Based on the rectangle method, replace the integral equation (1) with the following sum:

$$\sum_{i=1}^{n} K(x_i, y_j, s_l)z(y_j, s_l)\Delta s = u(x_i, y_j), \quad i = \overline{1,n}, \quad j = \overline{1,m}. \tag{4}$$

Rewrite (4) in the matrix form:

$$A\bar{z} = \bar{f}, \tag{5}$$

where $\bar{z} = \{z(y, s_l)\}_{l=\overline{1,n}}$ is the vector of unknowns, $\bar{f} = \{u(x_i, y)\}_{i=\overline{1,n}}$ is the right-hand side, A is the square matrix with elements

$$A = \{a_{il}\}_{\substack{i=\overline{1,n} \\ l=\overline{1,n}}}, \quad a_{il} = \frac{h\Delta s}{\pi(x_i - s_l)^2 + h^2}.$$

The main features of the (5) system are:

a) large dimension;

b) strong sparseness of the matrix Aand the right-hand side $\bar{f}$;;

c) bad conditioning.

Therefore, according to [17-19], the M. Lavrentiev regularization method is usedfor the numerical solution of the matrix equation (5):

$$\bar{A}\bar{z} = \bar{f}, \tag{6}$$

where $\bar{A} = \mu E + A$, $\mu > 0$ is a some parameter. To numerically solve the equation (6), the Landweber iteration method is used

$$\frac{\bar{z}^{k+1} - \bar{z}^{k}}{\tau} + \bar{A}\bar{z}^{k} = \bar{f},$$

where $\bar{z}^{k}$ is the value of $\bar{z}$ at the k-th iteration. The condition for the completion of the iterative process is the achievement of the inequality $\left\|\bar{z}^{k+1} - \bar{z}^{k}\right\|_{\infty} < \varepsilon$ for the given number ε.

Description of the software module of the geographic information system. Today, there are many multifunctional GIS implemented on the basis of web and desktop technologies (i.e. MapServer, MapFish, GeoMixer, ArcGIS, Google Maps API, QGIS). Each of these systems has some advantages and specific characteristics. Since 2010, the popularity of QGIS has been growing [20, 21], so in 2019, interest in QGIS was about two times higher than that of its proprietary counterpart — ArcGIS. QGIS supports all the most important Open Geospatial Consortium (OGC) specifications:

- WMS — Web Map Service (Client WMS/WMTS);
- WMTS — Web Map Tile Service (Client WMS/WMTS);
- WFS — Web Feature Service (Client WFS and WFS-T);
- WFS-T — Web Feature Service - Transactional (Client WFS and WFS-T);
- WCS — Web Coverage Service (Client WCS);
- SFS — Simple Features for SQL (Layers PostGIS);
- GML — Geography Markup Language.

OGC services are used for the exchange of geospatial data between various GIS and data warehouses. QGIS can be adapted to special needs with the help of an extensible module architecture that allows you to solve a variety of tasks from geocoding to geometry simplification, integration with web mapping services and 3D landscape modeling. In addition, QGIS allows software developers to expand the functionality of this platform with the help of dynamically connected custom software modules for solving specialized tasks. They are created using a software development kit in the C++ or Python programming languages.

The authors of thispaper have developed a software module for the QGIS system which provides QGIS users the necessary set of methods for restoring the distribution fields of chemical elements at a given depth, and has the following functionality:

1. Import of measurement input data from CSV files to the database;
2. Making predictive calculations based on the input measurement data and the algorithm for solving the inverse problem;
3. Visualization of the initial data and the data obtained as a result of solving the inverse problem.

The structure of the software extension consists of two parts. The first part is written in Python and represents program instructions for user interaction with the information system interface. The second part, the computational core, contains the implementation of algorithms for solving the inverse problem. Due to the relatively low speed of execution of programs written in Python, the question of choosing a suitable programming language is raised. Julia, a high-performance programming language for mathematical calculations, was chosen as such a language, in which the main emphasis is placed on computing performance. The standard package includes a JIT compiler based on LLVM, so that applications written entirely in the language are almost as good in performance as applications written in statically compiled languages, such as C or C++. A large number of libraries have been created for the Julia language, including for solving differential

equations, visualization, interaction with databases, and others. One of the priorities in the development of the language is the support of parallel and distributed computing. This decision on the structure of the software module was made due to the need to increase the performance of algorithms, the possibility of using the rich mathematical library of the Julia language, as well as for reusing the computational library for implementing extensions in other software environments.

The initial information is presented in CSV format files, which contain the geodetic coordinates of the sampling points, the depth of occurrence and the measurement values for 29 chemical elements. The object-relational database management system PostgreSQL is used to manage the initial geochemical, geophysical and geological information. The choice of a DBMS is primarily related to the possibility of indexing geometric objects and the presence of a PostGIS extension based on it.

The data is grouped into logically named data sets, which are called sessions. The concept of sessions allows considering data sets independently of each other, to separate them by the time of receipt and by origin. Several versions of the data of the same deposit can coexist in the database, which can be obtained not only as a result of sampling, but also as a result of computational experiments with different calculation parameters. Each session has a parent session based on which it was created.

Figure 1 shows a fragment of the database scheme used by the software module, which includes the following main tables:

1. “Session”, a table that stores data about sessions, including its name, date and time of its creation, a type, as well as the ID of its parent session;
2. “Chemicals” which stores the names of chemical elements;
3. “Chemdata”with the fields «Measurement depth», «Chemical element», «Sample sampling coordinates», «Measurement values»which stores the initial measurement data and calculation results;
4. «Sesstypes» which stores the names of session types.

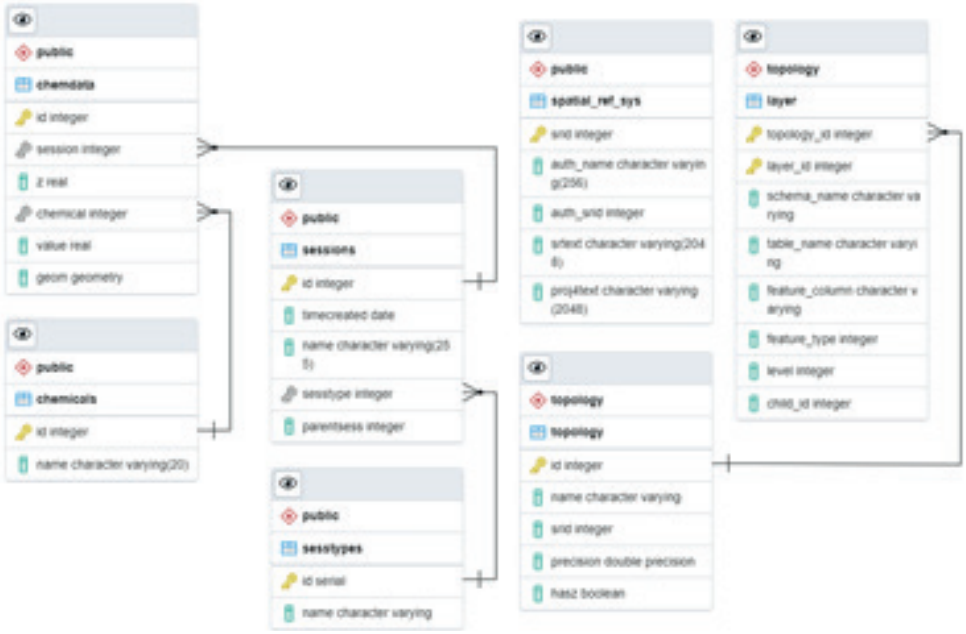


Figure1 – Fragmentof the database schema

The algorithm for the QGIS user actions to interact with the module’s functions is as follows. First of all, the user needs to upload the source data with the geodetic coordinates of the sampling points and the measurement values to the database. For this purpose, the possibility of automated parsing of sourceCSV files and importing information into the database using Python Pandas and psycopg2 packages is implemented.

At the second step, predictive calculations are performed to determine the distribution field of chemical elements based on the mathematical model (1)-(3). This functionality is implemented in the computing core, which contains the implementation of algorithms for solving inverse problems. The kernel allows one to accept problem parameters as arguments, so the program module can call this program with different input data. The computing core configuration dialog box allows one to set the following parameters:

1) Calculation grid configuration and theparent session;

2) The chemical element for which it is necessary to restore the field, and the depth;

3) Calculation parameters (regularization parameter, maximum number of iterations, calculation accuracy, iteration parameter value).

The next step is to visualize the data. After confirmation, an SQL query is dynamically compiled and the sample coordinates and measurement values (or values obtained as a result of calculations) are loaded. Based on the received information, a new vector layer with isolines of values is created. Topographic maps are used as a substrate, which are accessed via ArcGIS REST Services. The resulting map fragment with the visualization result can be exported to various graphic formats.

Verification of the software module. To verify the developed software module, a number of methodological calculations were carried out using data on the Novo-Khairuzovsky area of southern Altai [12]. The purpose of the computational experiments is to reconstruct the distribution field z_C of a given chemical element at a depth h according to the (1)-(3) model on the base of the known empirical data on the day surface, and also to compare the results obtained with the empirical data z_E at depth h obtained from field and laboratory studies. The results of computational experiments carried out for the chemical element gold are given below.

The proposed approach was tested on a grid of 201×201 nodes with $\mu = 0.5$, $\varepsilon = 10^{-6}$. Table 1 shows a fragment of data for several randomly selected points. The second column of the table contains the gold concentration values obtained as a result of the field research. This information is used as initial data for forecasting calculations using the model (1)-(3). The rest of the columns contain data from computational experiments z_E for depths from 100 to 400 meters and reference values from field and laboratory studies z_C.

Table 1 – Fragmentof data comparing the calculated values $z_C$of gold concentration at depth h with the values z_E obtained as a result of field and laboratory studies, $\bar{z} = |z_C - z_E|$

Abnormal point	h=0	h=100 m.		h-200 m.		h=300 m.		h=400 m.	
		z_C	z_E	z_C	z_E	z_C	z_E	z_C	z_E
1	0.0247	0.0314	0.0316	0.0392	0.0370	0.0396	0.0371	0.0309	0.0372
2	0.0221	0.0320	0.0319	0.0288	0.0312	0.0355	0.0323	0.0342	0.0297
3	0.0477	0.0711	0.0709	0.0694	0.0718	0.0668	0.0724	0.0532	0.0633
4	0.0192	0.0225	0.0240	0.0249	0.0267	0.0260	0.0273	0.0267	0.0268
5	0.0194	0.0255	0.0283	0.0288	0.0279	0.0299	0.0263	0.0302	0.0268
6	0.0220	0.0242	0.0267	0.0264	0.0292	0.0291	0.0349	0.0308	0.0316
7	0.0160	0.0199	0.0204	0.0215	0.0233	0.0228	0.0229	0.0242	0.0226
8	0.0228	0.0276	0.0295	0.0312	0.0330	0.0335	0.0324	0.0350	0.0319

The reliability of the calculation results was assessed by comparing the calculated values obtained within the framework of themodel (1)-(3) and the reference values of the gold concentration for the depth n. The following criteria were used for the assessment:

1) Average absolute forecast error:

$$\Delta\bar{z} = \sum_{i=1}^{n} \frac{z_C^{(i)} - z_E^{(i)}}{n},$$

where $\Delta\bar{z}$ is the mean absolute error in the concentration prediction, n is the number of points used for comparison, z_C is the gold concentration according to analytical data, z_E is the gold concentration according to the model data, the superscript denotes the corresponding value at the *i*-th point.

2) Root mean square forecast error (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(z_C^{(i)} - z_E^{(i)}\right)^2}.$$

3) The ratio of RMSE to the average reference concentration:

$$\delta_{\text{mean}} = \frac{\text{RMSE}}{\bar{z}}.$$

The analysis results are shown in Table 2.

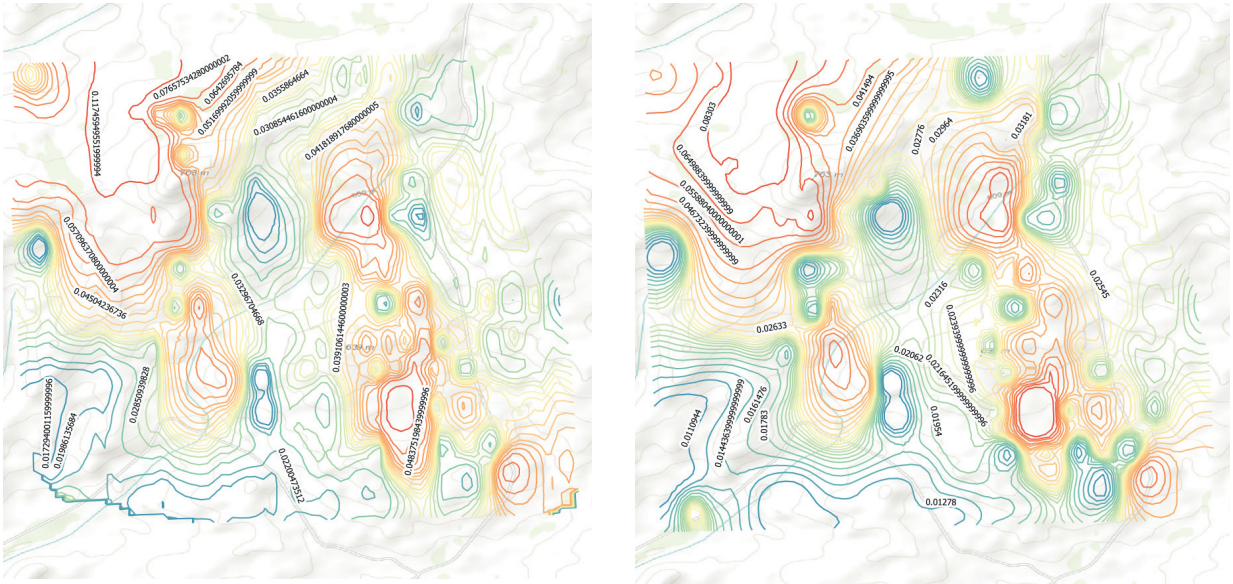
Table 2 – Assessment of the reliability of the calculated gold concentration

Criteria for assessing the reliability of the calculation	h=100 m.	h=200 m.	h = 300 m.	h = 400 m.
Average absolute forecast error	0.002797	0.002216	0.003856	0.009075
Root mean square forecast error	0.003001	0.002440	0.004349	0.010661
The ratio of RMSE to the average reference concentration	0.016860	0.019931	0.126216	0.198731

The rootmeansquare error in calculating the concentration according to the model at a depth less than h = 200 m is under 2% of the average empirical concentration value. Such errors can be considered acceptable. It can be assumed that themodel (1)-(3) allows one to fairly accurately reconstruct the distribution field of a chemical element. At a lower depth, the forecast RMSE sharply increases, up to 12.62% at h=300 m and up to 19.87% at h=400 m. The degree of deviation of the calculated concentration according to themodel (1)-(3) depends on the proximity of the primary source, the composition of the ores and the landscape-geochemical features of the hypergenesis zone (the degree of acidity and saturation with halogens of surface waters, draining deposits).

Figure 2 (a) shows the digital surface of the distribution of gold anomalies built in the QGIS geographic information system and based on the calculated data using the model (1)-(3) at a depth of $h = 300$ m. For comparison, Figure 2 (b) shows the digital surface based on the reference values.

Conclusion. Thus, the paper presents the results of developing a software module for the QGIS geographic information system, which implements algorithms for solving inverse problems to restore the distribution field of chemical elements at a given depth. The module also contains a number of auxiliary solutions to expand the functionality of this information system. A comparative analysis of the calculated data with empirical data carried out for the verification of the model shows that the model makes it possible to fairly accurately reconstruct the distribution field at a shallow depth, with an error of less than 2%. At a lower depth, the deviation of the calculated data from the reference data significantly increases, however, due to the ill-posedness of the inverse problems, the results obtained can also be considered acceptable. Further work will be aimed at improving the accuracy of the mathematical model.



a) calculated values b) reference values

Figure 2 – Comparison of gold concentrations at a depth of 300 m.

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МАТЕМАТИКАЛЫҚ МОДЕЛЬДЕУ ЖӘНЕ БОЛЖАУДЫҢ ЦИФРЛЫҚ ӘДІСТЕРІ НЕГІЗІНДЕ ГЕОХИМИЯЛЫҚ ӨРІСТЕРДІ ТАЛДАУҒА АРНАЛҒАН ГЕОАҚПАРАТТЫҚ ЖҮЙЕНІҢ МОДУЛІ

Аннотация: Бұл жұмыста кен орындарын терең іздестіру үшін аномалияларды интеллектуалдық анықтау әдістерін зерттеу шеңберінде әзірленген геоақпараттық жүйенің бағдарламалық модулінің сипаттамасы келтіріледі. Модуль Пуассон ядросы бар Фредгольм интегралдық теңдеуі мен берілген тереңдік техимиялық элементтің таралу өрісін анықтаудың математикалық моделін қолдануға негізделген. Бағдарламалық модуль күндізгі бетіндегі өлшеу деректері негізінде химиялық элементтер концентрациясының болжамды есептеулерін жүргізу үшін көрсетілген кері есепті шешу алгоритмдерін, сондай-ақ бір қатар көмекші мүмкіндіктерді іске асыруды қамтиды. Алгоритм М. Лаврентьевтің регуляризациялау әдісімен Ландвебердің итерация әдісін қолдану арқылы жүзеге асырылды. Болжамды есептеулердің географиялық байланыстырылған нәтижелері QGIS геоақпараттық жүйесінің картасында көрсетіледі. Жұмыста бағдарламалық модульдің құрылымы және оны әзірлеу процесі, сондай-ақ модуль функциялары мен өзара әрекеттесуге арналған QGIS пайдаланушысының әрекет ету алгоритмі сипатталған. Далалық және зертханалық зерттеулер нәтижесінде алынған бастапқы деректерді дерек қорға автоматты түрде импорттау жүзеге асырылды. Геоақпараттық жүйенің деректер базасында Қазақстан аумағында орналасқан Оңтүстік Алтайдың Жаңа – Хайрузовка учаскесі бойынша 3920 материал алу нүктесіндегі 29 химиялық элемент бойынша деректер бар. Математикалық модель алтын химиялық элементі бойынша алынған эмпирикалық деректер мен салыстыру арқылы сыналды. Салыстырмалы талдау негізінде келтірілген математикалық модель химиялық элементтердің таралу өрісін берілген тереңдікте жеткілікті дәлдікпен қалпына келтіруге мүмкіндік береді деген қорытынды жасалды.

Түйінді сөздер: геоинформатика, географиялық ақпараттық жүйе, географиялық ақпараттық жүйе модулі, барлау геохимиясы, математикалық модель.

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МОДУЛЬ ГЕОИНФОРМАЦИОННОЙ СИСТЕМЫ АНАЛИЗА ГЕОХИМИЧЕСКИХ ПОЛЕЙ НА ОСНОВЕ МАТЕМАТИЧЕСКОГО МОДЕЛИРОВАНИЯ И ЦИФРОВЫХ МЕТОДОВ ПРОГНОЗИРОВАНИЯ

Аннотация. В данной работе приводится описание программного модуля геоинформационной системы, разработанного в рамках исследований методов интеллектуального выявления аномалий для глубинных изысканий месторождений. Модуль основан на использовании математической модели определения поля распределения химического элемента на заданной глубине залегания, заданной интегральным уравнением Фредгольма с ядром Пуассона. Программный модуль содержит реализацию алгоритмов решения указанной обратной задачи для проведения прогнозных расчетов концентрации химических элементов на основе данных измерений на дневной поверхности, а также

ряд вспомогательных возможностей. Реализация алгоритма осуществлена с использованием метода регуляризации М. Лаврентьева и метод итерации Ландвебера. Результаты прогнозных расчетов отображаются на карте геоинформационной системы QGIS с географической привязкой. В работе описаны структура программного модуля и процесс его разработки, а также алгоритм действий пользователя QGIS для взаимодействия с функциями модуля. Реализован автоматизированный импорт исходных данных, полученных в результате полевых и лабораторных исследований, в базу данных. База данных геоинформационной системы содержит данные по 29 химическим элементам в 3920 точках забора материала по Ново-Хайрузовскому участку южного Алтая, расположенного на территории Казахстана. Проведена апробация математической модели посредством сравнения расчетных данных с эмпирическими данными для химического элемента золото. На основе проведенного сравнительного анализа сделан вывод о том, что математическая модель позволяет восстановить поле распределения химических элементов на заданной глубине залегания с приемлемой точностью.

Ключевые слова: геоинформатика, географическая информационная система, модуль геоинформационной системы, разведочная геохимия, математическая модель.

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