

Empowering geological data analysis with specialized software GIS modules

Dossan Baigereyev^{1,2}, Syrym Kasenov³, Laura Temirbekova^{1,4}

¹National Engineering Academy of RK, Almaty, Kazakhstan

²Sarsen Amanzholov East Kazakhstan University, Ust-Kamenogorsk, Kazakhstan

³Department of Computational Sciences and Statistics, Faculty of Mechanics and Mathematics, Al-Farabi Kazakh National University, Almaty, Kazakhstan

⁴Abai Kazakh National Pedagogical University, Almaty, Kazakhstan

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ABSTRACT

This research is devoted to the development of a geographic information system (GIS) for the analysis of geological data. It presents two specialized software modules designed to solve complex geological problems related to potential progress to disturbed masses and magnetotelluric sounding. These modules are integrated into the QGIS environment, offering efficient data processing and analysis capabilities, contributing to a deeper understanding of geological structures. The study presents a mathematical model for the problem of magnetotelluric sounding (MTS) and the continuation of potentials towards the perturbed masses, demonstrating numerical results using the developed algorithm. To confirm the accuracy of the model, a comparative analysis was carried out with empirical data for various chemical elements, which showed high accuracy, especially at shallow depths, with an error rate of less than 2%. In addition, the study highlights the importance of powerful GIS for the analysis and interpretation of geological data, including geochemical, geophysical and remote sensing information. The advanced functionality of QGIS simplifies data processing and visualization, which makes it an invaluable tool for geologists and researchers.

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Corresponding Author:

Syrym Kasenov

Department of Computational Sciences and Statistics, Faculty of Mechanics and Mathematics

Al-Farabi Kazakh National University

Almaty, Kazakhstan

Email: syrym.kasenov@gmail.com

1. INTRODUCTION

At the present stage of economic development, the increasing need for various types of mineral resources is becoming a stable trend. New territories are being involved in the processes of geological exploration, and infrastructure clusters are developing. In the medium term, mineral resources will continue to be the foundation of the socio-economic development of the countries of raw materials specialization, emphasizing the importance of objective geological and economic analysis, monitoring and accounting of minerals for forecasting promising areas of use. As a result, there is an urgent need to develop a system of permanent geological monitoring to assess the state of mineral resources and the potential of the territory [1]–[3]. Given the significant number of controlled parameters, data sources and computational algorithms in geological and economic research, it becomes necessary to develop a system architecture capable of providing high performance for various levels of use. At the same time, it is necessary to ensure the integrity of the information database and integration with geographic information mapping services. In this regard, in practice, the use of geographic information systems seems appropriate.

A geographic information system (GIS) is a set of application programs and tools designed to collect [4], [5], store, analyze and geographically visualize spatial data about the objects under study. This complexity includes database management systems, raster and vector graphics editing tools, as well as analytical capabilities. GIS is widely used in the field of cartography, geology, meteorology, ecology, land management, economics, municipal administration and many other related fields. The use of GIS greatly simplifies the analysis of multidimensional data using digital maps. This improves environmental forecasting procedures in resource extraction procedures, allows for an assessment of the complex impact on the natural environment and promptly identify anomalies to take appropriate measures [6], [7].

Map creation and geographical analysis are well-known methods. However, GIS represents a new, more modern and effective approach to analyzing problems and solving problems facing humanity. GIS automates analysis and forecasting, which was not available before. Today GIS is a modern territorial management tool based on modern information technologies and data from various sources, including aerial and space surveys, geographical maps and other geographically distributed data [8]–[10].

Significant funding is required for the discovery and development of new hidden deposits. The solution of such problems is not feasible without the widespread use of modern geoinformation methods for data analysis, as well as methods of mathematical geophysics and geochemistry. Within the framework of the scientific project AR14871252 “Construction and research of quaternion fourier transforms and their application in the creation of information systems for problems of geophysics and geochemistry”, an information platform was created that combines initial data on geochemical, geophysical, geological studies and remote sensing data of selected deposits [11].

In this research, the characteristics of the geological structure, stratigraphy, intrusive magmatism and tectonics of the Novo-Khairuzovsk ore object are considered in detail. These features were important in the process of creating the GIS module. A lot of data of various scales, which has been systematized, is available at this facility. To develop the GIS module, the data obtained in the expedition studies of geochemical, geophysical and geological information were organized in a database using the PostgreSQL database management system. Within the framework of the principles and methodology of geological prospecting, new digital data and nonstandard characteristics of the geological environment were used to predict and search for hidden ore and hydrocarbon deposits. The freely distributed cross-platform geoinformation system QGIS quantum geoinformation system was used to organize and visualize data in the GIS module [11].

The work discusses the GIS module, which describes intelligent methods for the study of geological objects. The developed module is based on mathematical models that characterize the propagation of chemical elements at the depth of the Earth. Mathematical models are described by an ill-posed problem Fredholm equation of the first kind. The considered ill-posed problem is numerically solved using regularizing algorithms [12]. The GIS module makes it possible to implement predictive calculations of the distribution of chemical elements using the surface data of the Earth [13], [14]. Some gradient methods and the Lavrentiev method are used as regularizing algorithms. The obtained numerical results are visualized with the corresponding coordinates on the digital map of the data [15], [16].

Also, based on the data obtained using remote sensing, another inverse problem related to magnetotelluric sounding (MTS) is considered [17], [18]. The general approach to the inverse problems of MTS is to reconstruct the physical characteristics of the earth’s crust based on data on physical fields measured on the Earth’s surface. The main purpose of this approach is to study the structure of the upper layers of the Earth’s crust and search for mineral deposits. The solution of the inverse problem of MTS makes it possible to determine a geophysical model (resistance) based on data on apparent resistance.

Inverse problems of magnetotelluric sensing often encounter incorrectness, which usually leads to low accuracy of solutions and increased sensitivity to noise in the input data. Usually, to cope with such difficulties, reformulation of the tasks is used. These inverse problems in the field of magnetotelluric sensing, as a rule, are nonlinear and have several possible solutions [17], [18]. To solve them, geophysicists often use regularization methods, including linearized approaches [19]–[27]. Using regularization and various methods, such as the gradient method [19]–[21], the method of differential evolution [20], the problems of economics [22], [23], epidemiology [24], and geology [25]–[27], are solved. Despite the development of methods for solving geological tasks, there are very few cases where models have been integrated into specialized software for application to real geological objects.

Within the framework of this study, the following works will be performed:

- Information system development: development of new functionality in the QGIS information system using the created modules and algorithms, in order to improve the analysis of geological data. Development and integration of two software modules specialized in solving complex problems of potential continuation towards perturbed masses and magnetotelluric sounding.
- Model of the MTS problem and the continuation of potentials towards the perturbed masses: demonstration of numerical results of the MTS model problem using the developed algorithm.

- Data processing and visualization: when various geological, geophysical, geochemical and remote sensing data are received, their numerical analysis will be carried out and the results will be clearly presented on digital maps using the developed algorithms.
- Mathematical model validation: the mathematical model will be tested to validation by comparing its calculated data with empirical data for various chemical elements.

This study will present the results related to the expansion of the QGIS and the development of software modules for solving complex geological problems. Approbation of the mathematical model and comparative analysis with empirical data confirms the accuracy and effectiveness of the methods, which will be useful for geologists and researchers working with data on geological structures at different depths.

2. METHOD

2.1. Module of the GIS for predicting chemical anomalies

Geochemical mapping is a vital technique in the exploration for minerals, facilitating the creation of graphical representations and digital maps showcasing the spatial distribution of chemical elements. These visualizations serve as valuable indicators for identifying potential mineral deposits. However, while numerous geochemical anomalies may arise, only a fraction of them are associated with commercially viable deposits. Therefore, it is imperative to conduct comprehensive analyses of chemical element dispersion and concentrations, adhering to principles of geochemistry, to accurately assess these anomalies.

As part of research efforts, GIS module has been developed that employs advanced anomaly detection methods, specialized in predictive modeling of deposits. This module has undergone rigorous testing on real geological formations of various compositions and scales. To address inverse problems effectively, we utilize the high-performance programming languages Julia and Python, and seamlessly integrate them into the QGIS environment Figure 1. Utilizing GIS tools capable of handling geological data is crucial for our study. Among these tools, QGIS stands out as one of the most widely used, offering competitive capabilities compared to industry leaders like ArcGIS. Its agility in version updates, flexibility for integrating custom libraries and modules, and ability to tailor information and computing environments for spatial data analysis make it an invaluable asset in our research endeavors.

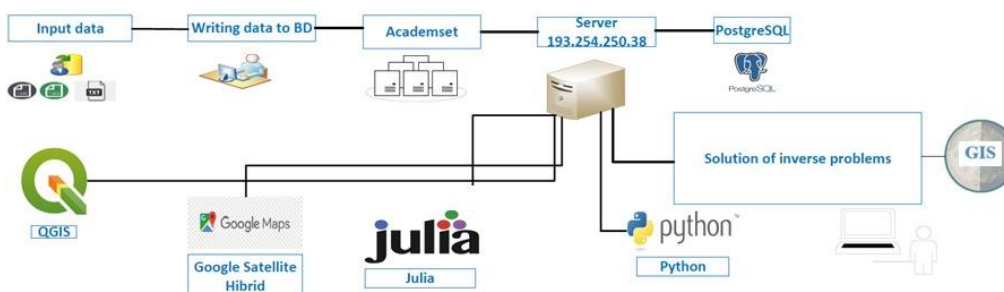


Figure 1. A model of the functioning of the QIS module in QGIS

Digital geological models typically originate from data collected through geophysical surveys conducted both in wells and on the ground. Within our GIS database, we have compiled extensive information regarding 29 chemical elements, obtained from 3,920 material sampling points located at the Novo-Khairuzovsk field in southern Altai, Kazakhstan. Managing this wealth of initial geochemical, geophysical, and geological data is facilitated by the use of the object-relational database management system PostgreSQL. Notably, PostgreSQL's capability to index geometric objects and its support for the PostGIS extension enhance data organization and retrieval.

The geological data within the database is organized into logically named datasets, as illustrated in Figure 2. Sessions are employed to segregate these datasets based on the time and source of data acquisition. This approach allows for independent consideration of datasets and facilitates differentiation between data originating from various sources. Additionally, the database accommodates multiple versions of data pertaining to the same deposit, which may stem from both physical sampling and computational experiments involving varied calculation parameters. Each session is linked to an original underlying session from which it was derived, ensuring traceability and continuity in data management. Figure 2 shows a fragment of the database used by the software module, which includes the main tables "sessions", "chemicals", "chemdata", "sesstypes" [11].

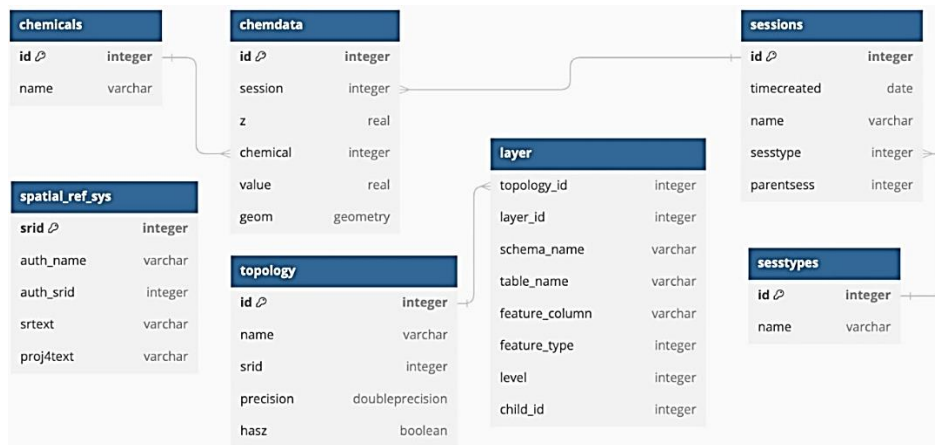


Figure 2. The database scheme of the created module in QGIS with logically grouped datasets

QGIS seamlessly integrates with critical open geospatial consortium (OGC) standards, facilitating the exchange of geospatial data across various GIS platforms and data repositories. Notably, QGIS offers the flexibility to enhance its capabilities through the integration of custom user software modules designed for specific tasks, which can be dynamically connected [11]. The uniqueness of the research lies in the fact that the functionality of QGIS is extended by two software modules that solve the problems of potential continuation in the direction of changing masses and magnetotelluric sensing. When geological, geophysical, geochemical and remote sensing data are received, the calculation is performed and the calculation results are visualized on a digital map.

2.2. Numerical solutions of the direct and inverse MTS problem

This paragraph demonstrates the numerical results of the MTS model problem. When remote sensing data is received, this algorithm is used to obtain results about the geological structure of the Earth. This algorithm is implemented in the QGIS module. The model problem consists of several horizontally homogeneous and isotropic layers Figure 3 with different properties: resistivity ρ_m and power h_m (where $m = 1,2,3$ is the layer number). The earth is divided into $n = 3$ horizontal isotropic layers with resistances ρ_1, ρ_2, ρ_3 and capacities h_1, h_2 . The power of the last layer (the third layer) is considered infinite. Each layer in this model is characterized by a magnetic permeability of $\mu_m = 1$. Main properties of given parameters are presented in [28]. In a direct problem, it is necessary to calculate the function ρ_T , which represents the apparent resistance. The reduced impedance is determined as (1).

$$R_1 = th \left(k_1 h_1 + arth \sqrt{\frac{\rho_2}{\rho_1}} \left[th \left(k_2 h_2 + arth \sqrt{\frac{\rho_3}{\rho_2}} \right) \right] \right) \tag{1}$$

Surface of the Earth		
Earth's crust	$\rho_1 = 100 \Omega \cdot m$	$h_1 = 1000 m$
Natural resource	$\rho_2 = 60 \Omega \cdot m$	$h_2 = 2000 m$
Earth's crust	$\rho_3 = 100 \Omega \cdot m$	$h_3 \rightarrow \infty$

Figure 3. The investigated model of the environment

Figure 4 shows a graph of the apparent resistance for this medium model. This graph demonstrates the correspondence of the reduced curve with the theoretical concepts of apparent resistance. It is noticeable that at high frequencies (small periods), the apparent resistance function depends on the upper layer, and as the period increases, we get information about the second and third layers.

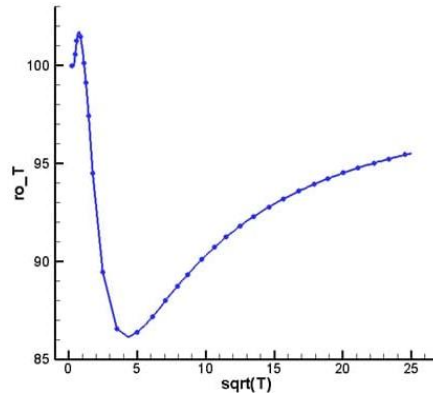


Figure 4. The investigated model of the environment

The inverse MTS problem involves a function of many variables, where some variables are fixed, such as the number of layers and the frequency of the incident wave, while other variables vary, such as the thickness of the layers and their resistivity. The goal of the inverse problem is to find the values of the power of the layers and resistivity, which minimize the sum of the squares of the deviations between the theoretical values of the apparent resistance modulus and the measured values for a given set of frequencies. Mathematically, the problem is formulated as (2) [27], [29], [30]:

$$J(q) = \sqrt{\sum_{i=1}^n (\hat{\rho}_T(\omega_i) - \rho_T(\omega_i, q))^2} \rightarrow \min \tag{2}$$

where $q = (\rho_1, \rho_2, \rho_3, h_1, h_2)$.

The MTS optimization problem is carried out using the differential evolution method. The main purpose of the method is to find the optimal values of system parameters to optimize certain properties of the system. Usually, the system parameters are represented as a vector. The objective function is a criterion that we strive to minimize in order to achieve an optimal solution. The method of differential evolution (DE) is one of the simple but effective algorithms for global minimization of the target functional [28], [31], [32]. The above algorithm numerically solves the multilayer inverse problem of MTS (2) with the data shown in Figure 5.

The image shown in Figure 5 shows that the proposed algorithm demonstrates a high convergence rate. The value of the functional is reduced to a very low level, about 10^{-22} , in just 275 iterations. From the analysis of the graph shown in Figure 6, it can be seen that at the first iteration, the apparent resistance graph deviates significantly from the exact solution. However, after 10 iterations, the graph begins to come close to the exact solution. After 100 iterations, the graph is almost identical to the exact solution, and at the last, 275th iteration, absolute convergence is achieved. This ensures that the environment value obtained at the last iteration fully corresponds to the true value. In comparison with the studies [29], the algorithm proposed by authors exhibits a higher convergence rate and provides significantly increased accuracy of the results.

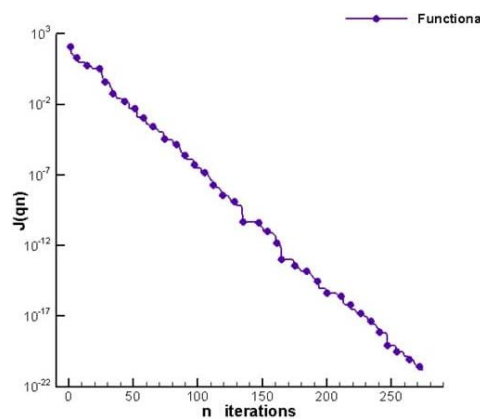


Figure 5. Graph of the functional $J(q_n)$ where $n = 275$

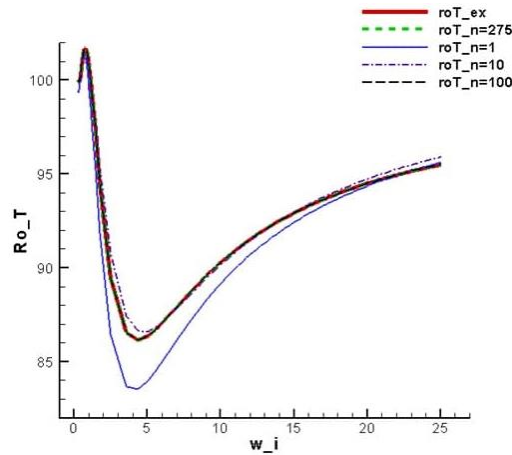


Figure 6. Change of the apparent resistance graph depending on the frequency in several iterations

In general, the differential evolution method is a very effective algorithm for global minimization of the target functional. It allows you to find optimal solutions to complex problems without numerous calculations and analytical expressions. The application of the differential evolution method can be especially useful in cases where it is difficult to calculate the gradient of the functional.

2.3. Solving the problem of continuation of potentials in the direction of changing masses

The developed software module utilizes a mathematical model as its core framework to analyze the distribution of a chemical element at a defined depth h . Within this model, the origin of the anomaly is determined using a flat model represented by the Fredholm integral equation with a poison kernel [8], [9]. This mathematical model forms the basis of our software module, enabling the assessment of the dispersion of a chemical element at a specified depth h . In this model, the origin of the anomaly is approximated through the utilization of a planar model, characterized by the integral Fredholm equation of the first kind, with consideration given to the poison kernel [6], [7]:

$$A(z) = \int_a^b K(x, y, s)z(y, s)ds = u(x, y), \quad y_{\min} \leq y \leq y_{\max} \quad (3)$$

$$z(y, a) = z(y, b) = 0, \quad z(c, x) = z(d, x) = 0 \quad (4)$$

here $u(x, y)$ represents the field that is already known at the ground or surface level, $z(y, s)$ signifies the field that is sought or desired at a depth h beneath the Earth's surface, $a = x_{\min}$, $b = x_{\max}$, $c = y_{\min}$, $d = y_{\max}$.

$$K(x, y, s) = \frac{h}{\pi(x-s)^2+h^2} \quad (5)$$

Issues (3) to (5) are part of the inverse problems category and represent an ill-posed problem. Given the challenges of obtaining an analytical solution for issues (3) to (5), this research turns to a numerical approach for resolution. Let's delve into a thorough examination of the numerical execution of (3). To initiate, the bounding rectangular area Ω is defined, encompassing a collection of points chosen for analysis on the Earth's surface.

Into the area Ω a homogeneous difference grid is introduced $\omega = \{(x_i, y_j), x_i = x_{\min} + i\Delta s, y_j = y_{\min} + j\Delta y, i = \overline{1, n}, j = \overline{1, m}, x_n = x_{\max}, y_m = y_{\max}\}$, where $\Delta s = (x_{\max} - x_{\min})/n$. Applying the rectangle formula, the integral (1) is replaced by the following sum:

$$\sum_{i=1}^n K(x_i, y_j, s_i)z(y_j, s_i)\Delta s = u(x_i, y_j), \quad i = \overline{1, n}, j = \overline{1, m} \quad (6)$$

In matrix form (6) is represented as in (7):

$$A\bar{z} = \bar{f} \quad (7)$$

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

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

The principal characteristics of the system (7) include substantial dimensionality, marked sparsity in both matrix A and the right-hand side \bar{f} , and significant ill-conditioning. Hence, following the recommendations in [26], [27], the numerical solution of the matrix (5) is computed using the regularization technique proposed by M. Lavrentiev:

$$\bar{A}\bar{z} = \bar{f} \tag{8}$$

here $\bar{A} = \mu E + A$, $\mu > 0$ represents a certain parameter. To calculate numerical solution of (8), 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} on the k th iteration. The iteration process is completed when the inequality $\|\bar{z}^{k+1} - \bar{z}^k\|_\infty < \varepsilon$ is fulfilled for a given number ε .

3. RESULTS AND DISCUSSION

3.1. Visualization of the results of inverse problems in the QGIS module

The QGIS module allows you to display on the map the initial data and the results of solving inverse problems according to the specified parameters (session and name of the chemical element). Before displaying the visualization dialog box, a list of recent sessions and a list of available chemical elements are loaded. After confirmation, a database query is generated dynamically. This query retrieves the coordinates of sampling and measurement values, or values acquired through computations. Subsequently, a new contour layer is generated on the map, displaying these values. The resulting map section with the visualization output can be exported in various graphical formats [33], [34].

To validate the developed software module, several methodological calculations were conducted using data from the Novo-Khairuzovsk section in southern part of Altai. The objective of these computational experiments is to reconstruct the distribution field of a specific chemical element, denoted as z_C , at depth h , utilizing a mathematical model grounded in empirical data collected from the Earth's surface. Subsequently, the obtained results are compared with empirical data, labeled as z_E , collected during field and laboratory studies. The results of these computational experiments, focusing on the chemical element gold, are provided.

The proposed approach was evaluated on a grid consisting of 201×201 nodes, with parameters set to $\mu = 0.5$ and $\varepsilon = 10^{-6}$. Table 1 presents a subset of data for several randomly chosen points. The second column of the table displays gold concentration values acquired from field research, serving as input for predictive calculations based on the mathematical model. Subsequent columns contain data resulting from computational experiments conducted at depths ranging from 100 to 400 meters (z_C), alongside reference values obtained from field and laboratory studies (z_E).

The accuracy of the calculation outcomes was evaluated through a comparison between the computed values derived from the model and the reference values of gold concentration at the specified depth Table 1. Criteria such as the average absolute error of the forecast and the standard error of the forecast were used for the assessment. In the process of calculating the degree of concentration, the standard error was less than 2% of the average empirical concentration. It has been based on the model at a depth of $h=200$ meters. We can infer that the model (3) to (5) enables the accurate reconstruction of the chemical element distribution field. However, at shallower depths, the forecast RMSE experiences a notable increase, reaching 12.62% at the depth of $h=300$ meters and 19.87% at the depth of $h=400$ meters. This deviation in calculated concentration, as per the model (3) to (5), is influenced by factors like the source proximity, ore composition, and the geochemical characteristics of the surrounding landscape, including surface water acidity and halogen saturation in areas draining mineral deposits.

In Figures 7 to 9, Figures 7(a), 8(a), 9(a) display the digital representations of zinc (Zn), copper (Cu), and gold (Au) anomaly distributions, respectively, in geology, when visualizing blue is used for zinc, green for

copper, and yellow for gold. Isolines and color saturation on the map indicate an increase in the concentration amount of the corresponding metal at the given coordinate. These representations were generated within the QGIS using computed data obtained from model (3) to (5) at depths ranging from 200 to 300 meters. By way of comparison, Figures 7(b), 8(b), 9(b) depict computer-generated surfaces derived from reference values.

Table 1. Data fragment with comparison of calculated values of z_C gold concentration at depth h with values z_E acquired through both fieldwork and laboratory analyses, $\bar{z} = |z_C - z_E|$

Abnormal point	h=0		h=100		h=200		h=300		h=400	
	z_C	z_E	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	0.037	0.0396	0.0371	0.0309	0.0372	
2	0.0221	0.0320	0.0319	0.0288	0.0312	0.0355	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	

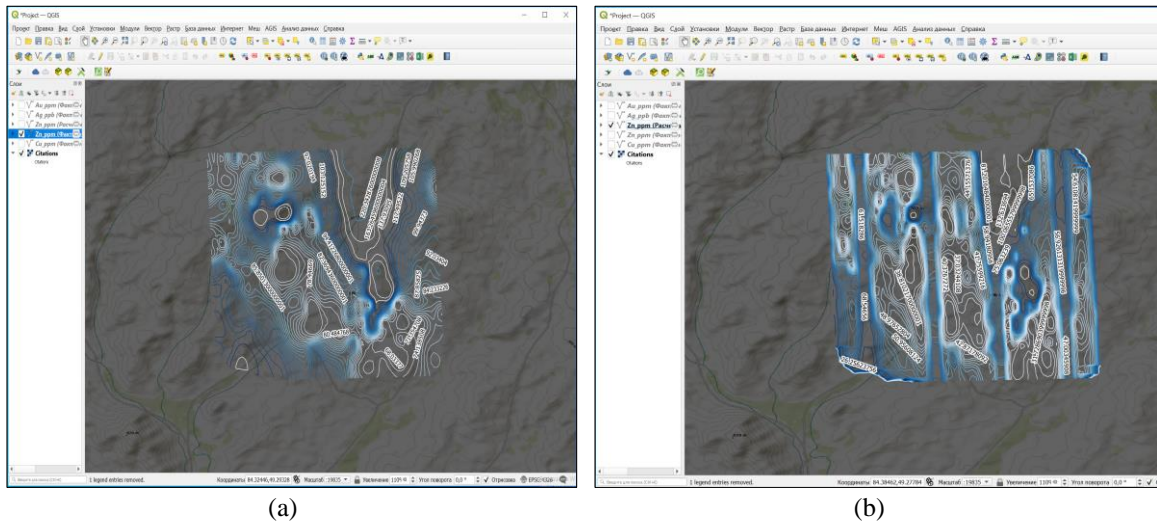


Figure 7. Visualization of the distribution of the chemical element Zn (zinc) on the daytime surface (a) at a depth of 200 meters and (b) using GIS

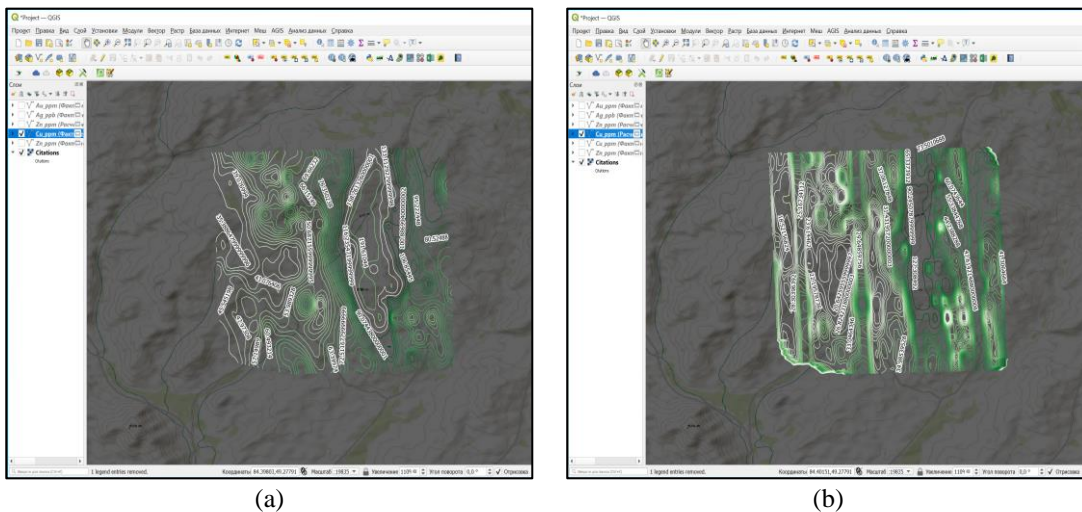


Figure 8. Visualization of the distribution of the chemical element Cu (copper) on the day surface (a) at a depth of 300 meters and (b) using GIS

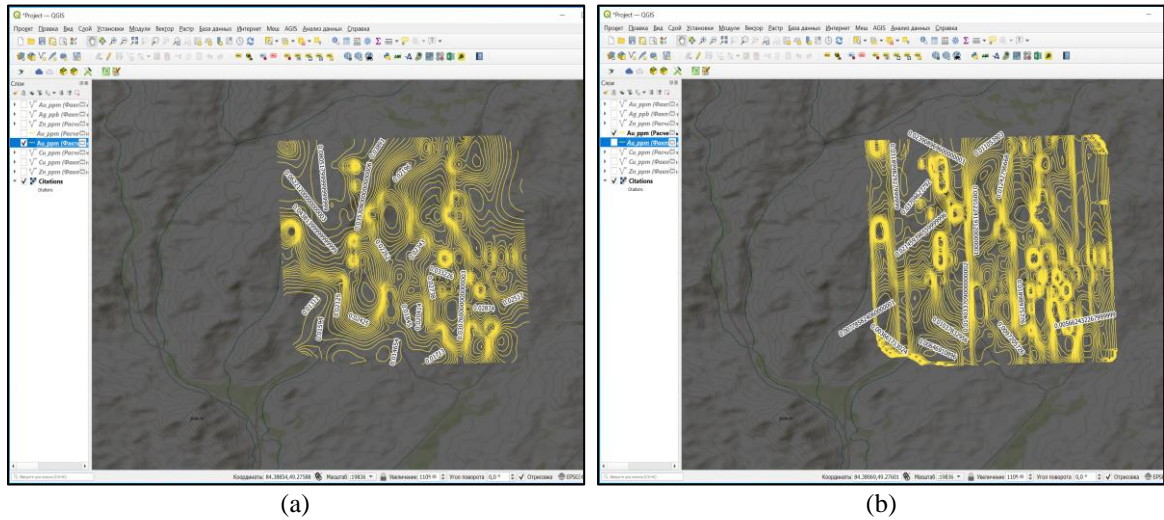


Figure 9. Visualization of the distribution of the chemical element Au (gold) on the day surface (a) at a depth of 200 meters and (b) using GIS

Figures 10 to 12 show the isolines of the distribution of the chemical elements zinc, copper and gold. Full information on the geochemical, geophysical and geological structure of the Novo-Khairuzovsk ore site, which were used in the development of the GIS module, is provided. From Figures 10 to 12, you can see the visualization of chemical elements without reference to geographical location, and in Figures 7, 8, 9, chemical elements are presented with a specific geographical location, which is very convenient for the user. The developed GIS can be used for any ore object, having the necessary input data.

Therefore, in this research there was presented results of creating a module of software within the QGIS. This module incorporates algorithms to solve inverse problems, aiming to reconstruct chemical elements dissemination at specified depths and MTS. Moreover, this module includes supplementary features that expand the capabilities of the geoinformation system.

To verify the considering model, a comparative analysis was conducted, aligning calculated data with empirical data. The results demonstrate that the model effectively reconstructs the distribution field at shallow depths with an error rate below 2%. As depth increases, the deviation between calculated and reference data also rises. Nevertheless, given the inherent challenges of inverse problems, the obtained results remain acceptable.

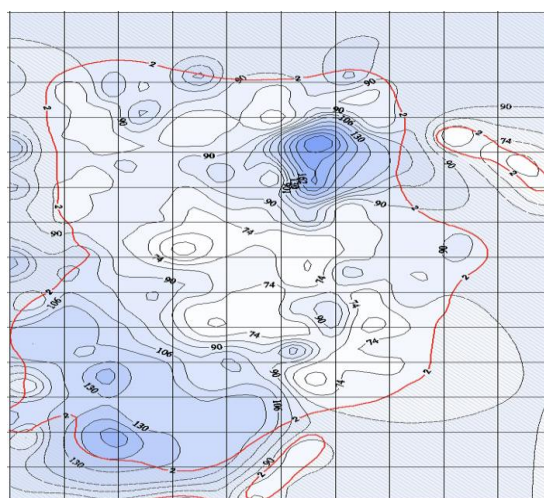


Figure 10. Generalized distribution model of the chemical element Zn (zinc) with a scale of 1:25,000

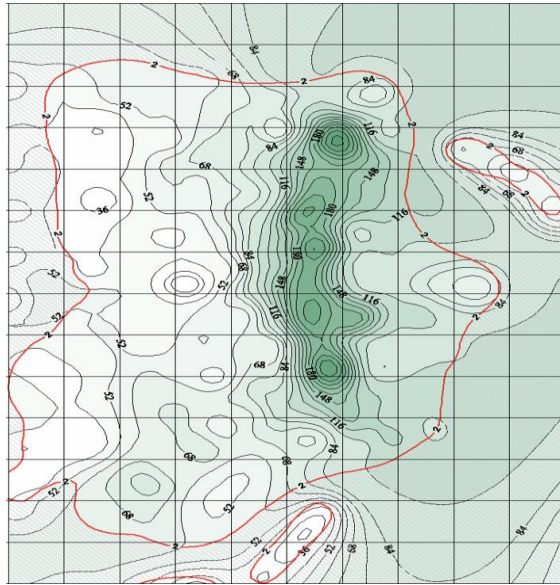


Figure 11. Generalized distribution model of the chemical element Cu (copper) with a scale of 1:25,000



Figure 12. Generalized distribution model of the chemical element Au (gold) with a scale of 1:25,000

4. CONCLUSION

In conclusion of this study, it should be emphasized that for the successful analysis and interpretation of geological data, including geochemical, geophysical and remote sensing data, the use of powerful geoinformation systems is required. As part of this study, the functionality of the QGIS environment was reviewed and expanded, allowing processing and visualizing this diverse array of data. One of the key aspects of the uniqueness of this study is the development of two software modules that are specialized in solving complex problems of potential continuation towards perturbed masses and magnetotelluric sensing. These modules are integrated into the QGIS environment, which allows analysts and researchers to efficiently process and analyze data for a deeper understanding of geological structures.

Throughout the research, a mathematical model was developed and tested, providing the foundation for assessing the chemical elements dissimination at specific depths. This model has been successfully used to analyze data obtained from a variety of sources, including geological, geophysical and geochemical studies. As a result of a comparative analysis between the calculated and empirical data, a high accuracy of the model was re-vealed, especially at shallow depths, with an error of less than 2%. This approach to solving MTS problems is effective, along with methods such as neural networks for solving inverse problems. This work can later be integrated into various geological exploration and research projects and programs, along with various geological technologies. This research project represents an important step in the development of geoinformation systems for geological research. New software modules and mathematical models improve the analysis and processing capabilities of geological data, making them more accurate and efficient. This will be useful for geologists, researchers and other specialists engaged in the study of the earth's crust and resources.

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BIOGRAPHIES OF AUTHORS

Dossan Baigereyev     Ph.D., Associate Professor, East Kazakhstan University. He received a bachelor's degree and master's degree in Mathematics at East Kazakhstan University in 2007 and 2009, respectively, and a Ph.D. degree at East Kazakhstan Technical University in 2017. His main area of research are computational fluid dynamics, finite element method, finite difference method, fractional order differential equations, and parallel computing. He can be contacted at email: dbaigereyev@gmail.com.



Syrym Kasenov     Ph.D., Associate Professor. He graduated from East Kazakhstan State University, faculty of Mathematics in 2004 and he received a master's degree in Mathematics in 2006. He received Ph.D. degree at Abai Kazakh National Pedagogical University in 2012. Research interests: numerical methods, inverse problem, ill-posed problems. He has more than 60 scientific papers, including 17 articles based on Scopus and Web of Science. She can be contacted at email: syrym.kasenov@gmail.com.



Laura Temirbekova     graduated from al-Farabi Kazakh National University, Faculty of Mechanics and Mathematics in 2007, and she received a master's degree in mathematics in 2009. She received Ph.D. from al-Farabi Kazakh National University in 2013. Her research interests are numerical methods for solving inverse and ill-posed problems. She can be contacted at email: laura-nurlan@mail.ru.