

Predicting volcanic activity and compositional content of effusive rocks. Geochemical modelling of the formation of mud volcano breccias organic moieties using artificial intelligence capacity

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Abstract

Nowadays, with the advent and development of artificial intelligence (AI) capabilities, it has become realistic to perform accurate modelling and make predictions on many physical, chemical, biological and geological processes occurring in nature, in living organisms, or carried out artificially, in field, laboratory and industrial circumstances. Basic and specialized computer software (SW) of AI, covering practically all the data accumulated during centuries by rich human experience and practice of experimentation, allow to provide final, almost reliable information about given objects and processes. Since this direction and approaches are still only at the initial stage of their development, it seemed appropriate to provide information about some computer programs that allow modelling natural processes. As an example, this paper presents the question of modelling the organic composition of volcanic rocks by means of available computer programs provided by the AI network. It seems that this information will be useful for readers, profile specialists and experts in solving such problems and will save them from long wandering through various internet resources.

Keywords: artificial intelligence; geochemical modelling; geoinformation systems; computer programs for modelling volcanic magmatic processes; computer programs for determining the compositional composition of mud volcano breccias.

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1. Introduction

Several years ago, two of our review articles were published in the journal *Azerbaijan Oil Industry*, dedicated to the discovery and analysis of nanocarbon structures in volcanic and sedimentary rocks [1, 2]. It was shown that fullerenes are found in solid rocks and sedimentary deposits from the Cretaceous-Paleogene, Permian, and Precambrian geological periods. A map of the regions where fullerenes were discovered was provided, along with data on their concentrations in the rocks. Hypotheses of both biogenic and abiogenic origins of fullerenes were supported. According to the "biogenic" theory, during prolonged processes of metamorphism of sapropel and terrestrial plant matter – which, as is known, occur under pressure and high temperatures — various allotropic carbon compounds, including fullerenes, are formed and accumulate in the mineral matrix. In the "abiogenic" interpretation, fullerene formation

occurs as a result of shock impacts from lightning strikes or celestial bodies (such as the Sudbury meteorite and carbonaceous chondrite meteorites) hitting the Earth's surface, as well as from large-scale forest fires. According to global research findings, the predominant type of fullerene found in natural objects is C₆₀. Less frequently, other forms such as C₇₀, C₇₄, C₇₈, C₈₄, and C₁₀₀ have also been identified. An analysis of methodological approaches to fullerene identification has shown that to reliably and accurately determine their content, special high-resolution physicochemical methods must be used. These include laser desorption/ionization and electron-impact mass spectrometry (SELDI, MALDI), high-resolution scanning electron microscopy (HRSEM), transmission electron microscopy (HRTEM), and, in some cases, high-performance liquid chromatography (HPLC).

Similar conclusions were drawn in the review of studies related to the detection and analysis of nanocarbon single-layer planar and tubular structures. It has been shown that graphene, carbon nanotubes (CNTs), and carbon nanofibers (CNFs) exist within various igneous and sedimentary rocks. They are formed in graphite globules of volcanic rocks, as well as in sedimentary formations where pressure, metallic catalyst particles, shear stresses, and time spans of millions of years compensate for the absence of high temperatures. Researchers have also conducted experimental laboratory simulations of natural processes, demonstrating the realistic possibility of forming carbon nanostructures through the pyrolysis of volcanic gases on lava-based catalysts, mechanical activation, and treatment of amorphous carbon or bituminous coal.

The review particularly emphasized that all prerequisites exist for the formation of carbon nanostructures during mud volcano activity: the ejection of deep-seated rocks from a hot volcanic center; methane as the primary carbon feedstock; catalytically active breccias containing transition metals and their oxides; and the combustion of methane in an oxygen-depleted environment.

Fullerenes and carbon nanotubes are among the brightest representatives of nanotechnology objects and find the widest application in almost all areas of natural sciences and materials science. Tens and hundreds of thousands of researches have been carried out on carbon nanostructures up to the present time, the most important scientific and practical results have been obtained, which allowed to change many known ideas about the properties of materials, laws of their transformation, artificial and natural processes, significantly expand the boundaries of human cognition in many areas of natural and technical sciences [3-5].

In recent years, there has also been a trend towards the creation and study of nature-like technologies, i.e. processes that mimic natural laws and phenomena in real life. Fullerenes and carbon nanotubes are synthesised on a laboratory and industrial scale, whereas analogues of such synthesis exist in nature. Volcanic activity, which is the object of this study, is a vivid evidence of this.

It should be noted that actual analytical implementation of research on the breccias of mud volcanoes in Azerbaijan has not been, and still is not, feasible due to the lack of high-resolution analytical equipment. In this context, the comprehensive computer software modules currently offered by Artificial Intelligence (AI) systems could allow for the necessary preliminary geochemical modeling of volcanic and sedimentary rock compositions without the use of complex analytical instruments [6-8].

Thus, we found it reasonable to explore the capabilities of computer modeling and, in this article, present to the reader general approaches, as well as the main pathways, resources, guidelines, and recommendations offered by AI in an interactive format. We believe that this information will be highly

useful for specialized researchers and professionals working in this field when addressing similar or related issues.

2. Methodological part

To forecast volcanic activity in general, a wide range of modern programs and technologies is used. These tools help geologists and volcanologists collect, analyze, and interpret data obtained from various sources such as satellites, sensors, geophysical surveys, and laboratory experiments.

1. Geographic Information Systems (GIS)

Geographic Information Systems (GIS) are software tools designed for collecting, storing, analyzing, and visualizing spatial data. Volcanologists use GIS to integrate various types of data, including topographic maps, geological layers, seismic observation data, and satellite imagery.

- ArcGIS is a powerful platform for spatial analysis that enables working with data from different sources (e.g., cartographic and satellite). Using ArcGIS, volcanologists can create volcano activity maps, analyze surface changes, make forecasts based on historical volcanic activity, and model the consequences of eruptions.
- QGIS is a free and open-source alternative to ArcGIS, allowing users to work with large datasets and model different scenarios. Volcanologists use QGIS for analyzing satellite images, mapping volcanic activity, and performing risk assessments.
- Seismic Modeling is used to study the seismic activity of volcanoes and to detect seismic waves that pass through magma chambers. Programs such as SEISAN allow for the analysis of data from seismometers to identify seismic signals related to magma movement or stress in the Earth's crust.

These methods allow researchers to study the dynamics of volcanic processes such as magma accumulation in chambers or pressure buildup, which is crucial for predicting the composition of future eruptions.

Modeling Volcanic Processes in Real-Time

Real-time volcanic activity models can predict eruptions, ash emissions, and lava flows.

- Vulcan is software designed for modeling volcanic activity. It is used to create 3D models of volcanoes, allowing for tracking lava flows, lava landscapes, and even ash eruptions. Vulcan models can help predict which types of rocks will be ejected during an eruption.
- Ash3D is a model for calculating and predicting the spread of volcanic ash in the atmosphere. It takes into account numerous factors, such as wind speed, temperature, and humidity, and can predict how far ash may travel.
- Prediction Algorithms are used to process data from seismometers, gas sensors, and satellites to predict the characteristics of future eruptions, including the type of volcanic rock that may be ejected.

These approaches are crucial for analyzing eruption dynamics and assessing their impact on the environment, population, and minimizing potential risks.

To forecast the compositional composition of volcanic rocks based on factors such as location, nature (mud or magmatic volcanoes), volcano activity (active or extinct), and other conditions, several programs and tools can be used. However, it is worth noting that most programs for modeling volcanic rock compositions are focused on physicochemical processes (temperature, pressure, magma cooling), while

accounting for geographical and geological factors generally requires a combination of various methods, including the aforementioned GIS and specialized models.

3. Models of Magmatic Processes

These programs model the chemical and physical processes occurring in the magma chamber, helping to predict the composition of volcanic rocks.

3.1 COMAGMAT – a specialized program for modeling magma crystallization. It is used to calculate changes in the chemical composition of magma during cooling and crystallization. COMAGMAT allows volcanologists to predict which minerals will form at various temperatures and pressures, which in turn helps to forecast the composition of erupted rocks.

- **Description:** This program models magma crystallization, helping to predict which minerals and rocks may form depending on temperature and pressure in the magma chamber.
- **Suitable for:** Predicting the composition of magmatic rocks, taking into account crystallization processes, which can be useful for analyzing volcanic rock compositions.
- **How to use:** Used for modeling the composition of magma as it cools, which can help understand the composition of rocks erupted by active volcanoes.
- **Download:** Free for scientific purposes. [COMAGMAT](#)

3.2 MELTS and pMELTS – these programs are used for thermodynamic modeling of magmatic processes. They are used to calculate phase diagrams and determine the temperatures and pressures at which certain changes occur in the composition of magma. MELTS allows for evaluating how the composition of magma changes during cooling or with changes in pressure. pMELTS is a modification designed for calculations at lower pressures, such as those for volcanoes located on Earth's surface.

- **Description:** MELTS and pMELTS are programs for thermodynamic modeling of magmatic crystallization processes, which can be used to predict the composition of magma under different conditions (temperature, pressure, magma composition).
- **Suitable for:** Determining the composition of volcanic rocks depending on temperature and pressure conditions.
- **How to use:** These programs can be used to analyze chemical processes in the magma chamber, helping to predict the composition of volcanic rocks. Although they do not directly account for the location of the volcano, results can be interpreted with geological data in mind.
- **Download:** Free for scientific purposes. [MELTS](#)

These programs help predict which minerals and rocks will form under various conditions, which is especially important for volcanoes that can change the composition of magma during their existence. Thus, MELTS / pMELTS and COMAGMAT are programs that will help forecast the composition of magmatic rocks, but for a more comprehensive approach that includes location and other geological data, integration with GIS platforms such as QGIS will be required. QGIS, in combination with geological data and volcano maps, will help account for parameters such as the nature of the volcano (magmatic or mud), its age, location, and activity for more accurate predictions of volcanic rock composition.

4. QGIS + Geological Data

- **Description:** QGIS is a free and open-source GIS platform that allows working with geospatial data. For analyzing the compositional makeup of volcanic rocks, QGIS can be used in combination with geological maps, volcano data, and other spatial data.
- **Suitable for:** Modeling and analyzing the composition of volcanic rocks with consideration for location, type of volcano (magmatic or mud), as well as its age and activity.
- **How to use:** Using GIS methods, one can analyze data about volcanoes, such as their type, age, location, and activity, to predict which rocks may be associated with a given volcano. Geological maps, activity maps, and other data can be overlaid for further analysis.
- **Download:** Free. [QGIS](#)

5. PyMELTS

- **Description:** This is the Python version of MELTS, which allows integrating magma composition modeling with other programs and analyzing the results in the context of various geological factors, such as the location of the volcano or its type.
- **Suitable for:** Modeling magma composition based on various parameters and conditions of volcanoes, including data on location and nature of volcanic activity.
- **How to use:** Programming in Python enables the use of MELTS models and adapting them to different scenarios, including volcanoes with various types of activity (magmatic or mud volcanoes).
- **Download:** Free. [PyMELTS](#)

6. Open Source Volcano Modeling

- **Description:** This includes several open-source projects that can be used to create models of volcanic activity and predict the composition of volcanic rocks. These projects incorporate data about location, type of volcanoes (mud or magmatic), and their activity.
- **Suitable for:** Modeling and analyzing the composition of volcanic rocks based on various parameters of volcanoes (types, activity).
- **How to use:** These projects can use GIS and magma process models to predict rock composition considering additional factors.
- **Download:** Examples can be found on platforms like GitHub.

Task Formulation: Determining carbon nanostructures in the composition of mud volcano breccias through AI-based computer programs.

The material is presented in the original dialogue with AI.

Query: Is it possible to determine organic components in the surface breccias of mud volcanoes through GIS system software?

AI's Response: The geochemical program COMAGMAT is designed for modeling crystallization and phase transitions in magmatic systems, calculating phase equilibria during magma cooling, and determining the mineral and chemical composition of magmatic rocks based on temperature, pressure, initial magma composition, and oxygen potential. It is typically used for basalts, andesites, and other silicate magmas. The program is not intended for analyzing organic compounds, as it operates

exclusively within the domain of magmatic, silicate systems where organics are either absent or destroyed by high temperatures.

For mud volcanoes and organic substances, different programs are needed, such as:

- PHREEQC (for geochemical calculations of aqueous solutions),
- Geochemist's Workbench,
- TOUGHREACT,
- PetroMod (for oil and gas).

3. Results and discussion

Detailed Information on the Resolution Capabilities of Recommended Programs:

PHREEQC (USGS)

- **Purpose:** Modeling chemical interactions in aqueous-mineral and gas systems, simulating exchange reactions (e.g., between organic matter and minerals); determining organic solubility based on pressure, temperature, pH, and solution composition.
- **Suitable for:** Modeling mud volcanoes.
- **Pros:** Free, powerful, flexible.
- **Resolution Capabilities:** PHREEQC can simulate complex aqueous and geochemical interactions at various pressures and temperatures, offering high flexibility in modeling geochemical processes, including organic-mineral exchanges in mud volcano systems.

Geochemist's Workbench (GWB)

- **Purpose:** Professional geochemical modeling (including aqueous-gas and organic chemistry). Covers gas systems (CH_4 , CO_2 , H_2S , etc.), organic matter + minerals.
- **Suitable for:** Modeling mud and hydrothermal volcanoes.
- **Pros:** Visual interface, easy to use.
- **Resolution Capabilities:** GWB offers comprehensive tools for simulating both organic and inorganic geochemical processes with robust support for gas and aqueous interactions. Its resolution is highly dependent on the system being modeled but is generally high due to its focus on accurate modeling of complex geochemical systems.

TOUGHREACT (from Lawrence Berkeley Lab)

- **Purpose:** Modeling geochemical processes in porous media (including organic material and fluids), taking into account the migration of organic matter, heat flow, pressure, and gas phases.
- **Suitable for:** Modeling organic migration in geological media, including mud volcanoes.
- **Pros:** Specialized in porous media and fluid migration.
- **Resolution Capabilities:** TOUGHREACT is capable of simulating complex interactions between organic compounds, fluids, and porous media at high resolution. It handles geochemical reactions and fluid dynamics in geological formations with a focus on high-temperature and pressure environments, making it highly suitable for the study of mud volcanoes and organic migration.

PetroMod (Schlumberger)

- **Purpose:** Used for modeling hydrocarbon generation and migration, showing the formation of oil and gas, as well as their migration pathways in volcanic structures.
- **Suitable for:** Modeling oil and gas formation in volcanic systems.
- **Pros:** Advanced, primarily used in the oil industry, commercial license required.
- **Resolution Capabilities:** PetroMod offers high-resolution modeling, particularly for the oil and gas industries. It excels in simulating complex migration patterns, hydrocarbon generation, and the behavior of fluids within geological structures. Its application in volcanic systems offers insights into the migration of hydrocarbons, though the software is primarily designed for the petroleum industry.

Information on the Cost of Paid Programs

1. The Geochemist's Workbench (GWB)

GWB offers several versions with different features:

- **Essentials:** Around \$749.
- **Standard and Professional:** Prices are higher, but exact amounts are not listed on the official website.
- **ChemPlugin SDK:** \$639 for 3 months or \$1699 per year.
- Since 2023, GWB has transitioned to a subscription model, discontinuing lifetime licenses. Available subscriptions are 3-month and yearly.

2. PetroMod (Schlumberger)

PetroMod is industrial software for modeling oil and gas systems. Pricing is not publicly available and is provided upon request. To obtain pricing information, it is recommended to contact a Schlumberger regional office or an official representative.

4. Conclusion

1. Computer Programs for Predicting Volcanic Activity and Composition of Volcanic Rocks:

There are various software tools developed, especially in the context of Artificial Intelligence, for this purpose:

- **ArcGIS, QGIS, SEISAN, Vulcan, Ash3D:** For spatial analysis of volcanic states (phases of dormancy and activity, ash emission monitoring).
 - **COMAGMAT, MELTS, pMELTS, QGIS, PyMELTS, Open Source Volcano Modeling:** For modeling magmatic processes and volcanic rock composition.
 - **PHREEQC (USGS), Geochemist's Workbench (GWB), TOUGHREACT (Lawrence Berkeley Lab), PetroMod (Schlumberger), and also QGIS, Python version of MELTS, Open Source Volcano Modeling:** For modeling mud volcano activity and the compositional makeup of breccia deposits.
- ### **2. Determining Carbon Nanostructures in the Composition of Breccia in Mud Volcanoes:**
- The most productive methods for this analysis can be achieved using Geochemist's Workbench and PetroMod.

3. Brief Description of Specific Tasks:

The programs mentioned above are used for various tasks including:

- Predicting volcanic activity and volcanic rock composition.
- Modeling magmatic processes and composition of mud volcanoes and breccia formations.
- Access and usage details, including pricing and available subscriptions, are outlined for each software tool.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research

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