As a manuscript

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CRUSTAL STRUCTURE, THERMAL REGIME, AND HYDROCARBON POTENTIAL OF THE VOLGO-URALIAN SEGMENT OF THE EAST EUROPEAN CRATON

Specialty 1.6.9 – Geophysics

THESIS SYNOPSIS

for a degree of

candidate of geological and mineralogical sciences

Kazan - 2023

The work was carried out at the Department of Geophysics and Geoinformation Technologies of the Institute of Geology and Oil and Gas Technologies of the Kazan (Volga Region) Federal University.

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The defense will take place on May 4, 2023, at 14:00 at a meeting of the dissertation council KFU.016.2 at the Kazan (Volga Region) Federal University at the address: 420008, Kazan, St. Kremlevskaya, 4/5, Institute of Geology and Oil and Gas Technologies of KFU.

The dissertation can be found in the Scientific Library. N.I. Lobachevsky Kazan (Volga Region) Federal University (Kazan, st. Kremlevskaya, 35). Information about the defense, electronic versions of the dissertation and abstract are available on the official websites of the Higher Attestation Commission under the Ministry of Education and Science of the Russian Federation (https://vak.minobrnauki.gov.ru/) and Kazan (Volga Region) Federal University (http://kpfu.ru/).

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Abstract sent on "___" ___________ 2023

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GENERAL CHARACTERISTICS OF WORK

Relevance of the research topic.

The study of the structure of the Earth's crust, its thermal regime and their influence on the oil and gas content is a relevant task of modern geology and geophysics. First, this is due to the development of modern geophysical methods for studying the structure of the Earth's crust and upper mantle. One of the key methods, the development of which has undergone a qualitative leap in the last two decades, is satellite gravimetry. The advantage of this method is the complete and uniform coverage of the globe by satellite measurements of the gravity field with a resolution sufficient for a regional assessment of the structure of the Earth's crust. At the same time, the structure of the Earth's crust and upper mantle is interconnected with their thermal field [Artemieva, 2019; Lösing, Ebbing, Szwillus, 2020], which in turn affects the maturation of oil source rocks and, as a result, the oil and gas content of sedimentary basins [Beardsmore, Cull, 2001; Hantschel, Kauerauf, 2009]. This justifies to the use of satellite gravimetry data in the regional forecast of oil and gas content.

The task of constructing regional models of the Earth's crust using the inversion of the satellite gravity field is of great importance for the Russian Federation for two main reasons. First, at the moment in Russia, studies of the structure of the Earth's crust using satellite gravimetry data are not carried out so often. Secondly, Russia is still rich in territories whose hydrocarbon potential is not sufficiently discovered, such as the zone of the Arctic shelf. Given the insufficient degree of geophysical knowledge of the explored territories, the analysis of satellite gravimetry data can serve as the first step towards a more detailed study of their structure.

One of the promising regions of the Russian Federation for a pilot study of the structure of the Earth's crust based on satellite gravimetry data, as well as the study of the thermal regime and their influence on oil and gas potential, is the Volga-Ural hydrocarbon bearing province, which covers the eastern part of the Russian plate and the Cis-Ural foredeep [Lozin, 2002]. This region has a high degree of geological and geophysical knowledge, which is expressed, among other things, in the presence of seismic data partly revealing the deep structure of the Earth's crust, as well as in a long history of borehole geothermal measurements. At the same time, there is still an active discussion about the processes of oil maturation and migration in many large oil and gas fields in this region. Thus, the study of the structure of the Earth's crust in Volgo–Uralia and subsequent geothermal modeling is an important task that can shed light on the relationship between the spatial distribution of oil and gas content, the structure of the Earth's crust, and the heterogeneity of its thermal parameters.

The degree of research topic development.

At the present time, the possibility of using satellite gravimetry to study the structure of the Earth's crust, both globally and regionally, has been shown by many studies. An example of a global model of the Moho boundary structure is the GEMMA model built on the basis of GOCE satellite data [Reguzzoni, Sampietro, 2015]. Examples of regional models of the Earth's crust obtained as a result of satellite gravity data inversion are the models of the Earth's crust of Egypt [Sobh et al., 2019], Greenland [Steffen, Strykowski, Lund, 2017], Australia [Aitken, Salmon, Kennett, 2013] , Iran [Eshagh, Ebadi, Tenzer, 2017], South America [Meijde van der, Julià, Assumpção, 2013], the Asian orogenic belt [Guy, Holzrichter, Ebbing, 2017] and many other areas [Braitenberg, Ebbing, 2009; Haas, Ebbing, Szwillus, 2020; Jiang, Jin, McNutt, 2004; Singh, Rao, 2021; Welford et al., 2010].

The structure of the Earth's crust in the Volga-Ural region has been studied so far using field potential and seismic methods. So, G.E. Kuznetsov made a significant contribution to the studies of the structure of the Moho boundary within the Russian Plate in general and Tatarstan in particular using gravimetric data [Kuznetsov, 2002; Kuznetsov and Borovsky, 2000]. M.V. Mints et al. developed a model of the East European Craton (EEC), which includes a detailed description of the structure of its Volgo-Uralian segment, based on the TATSEIS-2003 depth seismic profile data (Mints et al., 2010). I. M. Artemieva and G. Thybo have created a model of Europe, Greenland, and the North Atlantic region EUNAseis. This model also includes the Volga-Ural region and was built exclusively from seismic data (Artemieva, Thybo, 2013). Additionally, it is necessary to highlight the fundamental works of S.V.

Bogdanova and A.V. Postnikov on the study of the material composition of the Earth's crust in the Volga-Ural region [Bogdanova, 1986; Postnikov, 2002].

The work on the study of the thermal regime of Volgo–Uralia has been actively carried out since the second half of the 20th century [Bulashevich, Shchapov, 1978; Neprimerov, 1971; Sinyavsky, Neprimerov, Nikolaev, 1978], when a large-scale program for measuring the heat flow was carried out. As a result, more than 800 measurements of the surface heat flow on the territory of the European part of the USSR were published [Lyubimova et al., 1973; Deep heat flow of the European part of the USSR, 1974]. One of the first models of temperature distribution within the sedimentary cover of the Volga–Ural region and the crystalline basement of Tatarstan was published by N.N. Khristoforova based on many years of work [Khristoforova, 2002; Khristoforova et al., 2004; Khristoforova, Khristoforov, Bergemann, 2008]. At the same time, the issue of lateral variations of the thermal parameters of Volgo–Uralia has not been fully disclosed, except for the work of A.A. Lipaev and others on thermal conductivity [Lipaev, Gurevich, Lipaev, 2001] and N.S. Boganik, V.N. Glaznev and others, and E.A. Lyubimova and others on radiogenic heat production (RHP) [Boganik, 1975; Glaznev et al., 2021; Lyubimova, Lyuboshits, Parfenyuk, 1983].

Previous studies of the relationship between the oil and gas content of Volgo–Uralia and the structure of the Earth's crust pay great attention to the faults of the Earth's crust as a factor influencing the location of oil and gas fields [Postnikov, 2002; Trofimov, Goryunov, Sabirov, 2017]. There is often a discussion about the possible role of crustal faults as hydrocarbon (HC) replenishment zones through degassing of the crystalline basement [Muslimov, Plotnikova, 2019; Plotnikova, 2008]. Nevertheless, the influence of the structure of the Earth's crust on oil and gas potential through the thermal field of the lithosphere has not been practically considered, despite significant work on the study of temperature distribution in wells in the Volga region [Khristoforova, 2002; Khristoforova et al., 2004; Khristoforova, Khristoforov, Bergemann, 2008].

Thus, at the moment, there are no studies of the structure of the Earth's crust within the Volga-Ural region based on modern satellite gravimetry data. Also, no work has been carried out on geothermal modeling taking into account the structure of the Earth's crust and lateral variations in thermal parameters. The question of the connection between the structure of the Earth's crust and the oil and gas potential of Volgo–Uralia, which manifests itself through the thermal regime of the lithosphere, remains unexplored.

Purpose and objectives of the study.

The main goal of the dissertation research is to determine the structure of the Earth's crust, the thermal regime, and their influence on hydrocarbon potential of the Volgo-Uralian segment of the EEC through the analysis of satellite gravimetry data and geothermal studies in wells.

To achieve this goal, the following tasks are to be solved:

1. Study the tectonic structure of the Volgo-Uralian segment of the EEC.
2. Collect the necessary geological and geophysical data for building a model of the Earth's crust of the region and subsequent geothermal modeling.
3. Carry out an inversion of the satellite gravity gradient field with a preliminary estimate of the Moho depth in the study area.
4. Create a three-dimensional density model of the Earth's crust and upper mantle of Volgo–Uralia by forward gravity modeling.
5. Carry out a statistical analysis of the geothermal structure of Volgo–Uralia using the previously obtained crustal model and the available data on the thermal field of the region under investigation.
6. Identify the main regularities of the relationship between the oil and gas content of the Volga-Ural oil and gas field and variations in the structural and thermal parameters of the Earth's crust and upper mantle of the region.
7. Determine directions for further work regarding clarifying the structure of the Volgo–Uralian crust, variations of its thermal properties, and assessing the hydrocarbon potential of the Volgo-Uralian segment of the EEC.

Scientific novelty of the research.

1. For the first time, satellite gravity data were used to model the crustal structure of the Volgo-Uralian segment of the EEC.
2. A new model of the Volgo–Uralian crustal structure has been built using satellite gravity and deep seismic data in the study area.
3. The modeling of the geothermal structure of the Volgo-Uralian segment of the EEC was carried out using the statistical Bayesian approach by the Markov Chain Monte Carlo method based on the previously created structural model.
4. For the first time, lateral variations of such thermal parameters of Volgo–Uralia as crustal thermal conductivity and radiogenic heat production, mantle thermal conductivity and mantle heat flow are calculated.
5. The main correlation patterns between the structural and thermal parameters of the Earth's crust and upper mantle, and the hydrocarbon potential of the Volga-Ural region are revealed.

Theoretical and practical significance of the work.

In the course of the work, a map of the Moho boundary was built, which is consistent with the gravitational field and seismic data on the structure of the Earth's crust in Volgo–Uralia. In the process of gravity modeling, the hypothesis of dense lower crust presence in the lower crust of the central Volgo–Uralia, corresponding to the so-called "Vetluga synform" has been confirmed [Mints et al., 2010; Artemieva and Thybo, 2013].

Modeling of the Volgo–Uralian geothermal structure made it possible to estimate the spatial variations in the crustal and upper mantle thermal parameters. A spatial relationship was revealed between radiogenic heat production and the distribution of Archean complexes of metasedimentary rocks of Volgo–Uralia, which, as was shown by A.V. Postnikov, also correlate with the distribution of oil fields in the territory of Volgo–Uralia (Postnikov, 2002). Based on the inversion results, a hypothesis was proposed about the increased radiogenic heat production of metasedimentary rocks of the Volga-Ural crystalline crust as a key factor influencing the heterogeneity of the Volga-Ural thermal field, which also potentially affects the maturation of oil source rocks.

From a practical point of view, the obtained models of crustal structure and thermal regime of Volgo–Uralia can be used to determine the rheological state of the lithosphere, as well as for basin analysis and modeling of hydrocarbon systems in order to assess the degree of maturity of oil source strata and perform further hydrocarbon deposits exploration.

Methodology.

To achieve the goal of the dissertation and solve the set tasks, the following methods were used:

1. Collection and digitization of the necessary data on the crustal structure and the thermal regiome of Volgo–Uralia.
2. Calculation of the gravitational effect of the sedimentary cover taking into account the curvature of the Earth using the tesseroid model and excluding this effect from the topographically corrected gravity gradient field [Uieda, Barbosa, Braitenberg, 2016].
3. Solution of the inverse problem of gravimetry using the technique of P. Haas et al. to consider the laterally changing density contrast between the Earth's crust and the mantle [Haas, Ebbing, Szwillus, 2020].
4. Forward gravity modeling in IGMAS+ software with simultaneous consideration of gravimetric measurements and seismic data on the crustal structure [Götze, Lahmeyer, 1988; Schmidt et al., 2020].
5. Numerical modeling of the thermal parameters' distribution of the Earth's crust and upper mantle based on the Bayesian approach using the Markov Chain Monte Carlo Method by analogy with the study [Lösing, Ebbing, Szwillus, 2020].
6. Testing the statistical hypotheses: on the normality of distribution according to the Shapiro-Wilk test [Shapiro, Wilk, 1965], on the homogeneity of variances according to the Levene test [Brown, Forsythe, 1974; Levene, 1960], on the difference in means according to Student's T-test [Gmurman, 2004; Kremer, 2010] for the statistical evaluation of the structural and thermal parameters of the Earth's

crust and upper mantle obtained in the process of modeling inside and outside the existing hydrocarbon fields.

All work on modeling and visualization of the crustal structure was carried out using the following software: ArcGIS Pro, Surfer, IGMAS+, Python programming language with an additional module for calculating the gravitational effect of tesseroids "Tesseroids" [Uieda, Barbosa, Braitenberg, 2016], a module for visualization spatial data PyGMT [Uieda, Leonardo et al., 2021] and a module for visualizing mathematical plots Matplotlib [Hunter, 2007]. The inversion of the satellite gravity gradient field to determine the Moho depth was carried out using the code of P. Haas et al. [Haas, Ebbing, Szwillus, 2020]. For Bayesian analysis of the thermal field and visualization of the results, the Python programming language was used with an additional module for visualizing statistical graphics Seaborn [Waskom, 2021], as well as the PyGMT and Matplotlib modules. The code of M. Lösing et al. [Lösing, Ebbing, Szwillus, 2020] was used as the basis for the Bayesian analysis. The SciPy module [Virtanen et al., 2020] was used to statistically analyze the difference in the values of the obtained structural and thermal parameters of the Earth's crust and upper mantle inside and outside the Volga-Ural hydrocarbon fields.

Provisions submitted for defense.

1. In the central part of Volgo–Uralia, a layer of high-dense lower crust was identified, confirming the hypothesis of magmatic underplating around the Vetluga synform, which was shown by the results of building a 3-D crustal model of the Volga-Ural region based on satellite gravimetry data.
2. It has been established that the use of a single-layer crustal model with vertically constant radiogenic heat production and thermal conductivity is a sufficient approximation for regional studies of the geothermal structure of the Archean cratons, which was shown by the results of geothermal modeling of Volgo–Uralia.
3. The main factor responsible for the spatial inhomogeneities of the surface heat flow of Volgo–Uralia, the radiogenic heat production of the Earth's crust, has been identified. There is a spatial correlation between areas of increased radiogenic heat production and the areas of high-aluminous metasedimentary rocks of the Bolshecheremshanskaya and other series, which, in turn, are associated with the location of large hydrocarbon fields in the region.

The degree of reliability and approbation study results.

The reliability of the models and conclusions proposed by the author is based on the control of the obtained models with the available a priori data and other similar models. To control the reliability of the lithospheric model of Volgo–Uralia obtained as a result of solving direct and inverse problems of gravimetry, both the available global and regional models of the Earth's crust and data from deep seismic studies were used. To control the reliability of the obtained geothermal model, we used data from temperature measurements in nine deep wells [Khristoforova, 2002; Khristoforova et al., 2004], as well as a temperature map at a depth of 1000 m in the Volga region [Khristoforova et al., 2004].

The main provisions and results of the study were reported at the International and National conferences: 73rd International Youth Scientific Conference "Oil and Gas 2019" (Moscow, 2019), 21st Conference on Geological Exploration and Development of Oil and Gas Fields "Geomodel 2019" (Gelendzhik, 2019), International Multidisciplinary Scientific GeoConference: "SGEM" (Vienna, Austria, 2020), 81st Conference of the German Geophysical Society (Annual meeting of the German Geophysical Society) (Kiel, Germany, 2021), General Assembly of the European Geophysical Union (EGU General Assembly) (Vienna, Austria, 2021), International Scientific and Practical Conference "The European Union's decision on decarbonization and a new paradigm for the development of the fuel and energy complex of Russia" (Kazan, 2021), IV All-Russian school-conference with international participation of students, graduate students and young scientists "Materials and Technologies of the XXI century" (Kazan, 2021), 82nd Conference of the German Geophysical Society (Munich, Germany, 2022).

The dissertation materials were published in 7 scientific papers: 5 in peer-reviewed scientific publications and recommended in the dissertation council of KFU in the specialty 1.6.9 "Geophysics". Among the published works 6 are indexed in Scopus, 4 in WoS, 2 are published in journals recommended by the Higher Attestation Commission under the Ministry of Science and Higher Education.

Structure and scope of work.

The dissertation consists of an introduction, four chapters, a conclusion, a list of references, including 270 titles, illustrated with 45 figures and 11 tables. The total volume of work is 146 pages.

Personal contribution of the author to the solution of the set tasks.

The dissertation is based on the author's independent research and consisted of collecting, digitizing, analyzing, modeling, interpreting and visualizing data. In the process of working on the dissertation, the author carried out the following work:

1. The general scientific literature on current ideas about the structure of the Earth's crust and upper mantle and methods for its study, satellite gravimetry, heat flow, basin analysis, and features of the crustal structure in oil and gas areas was analyzed. In addition, the scientific literature on the heat flow, tectonic structure, and evolution of the Volgo-Uralian segment of the EEC and the history of geothermal research in this region was analyzed.
2. The necessary geological and geophysical data have been collected to build a crustal model of the region, which includes the satellite gravity and gravity gradient fields, topography, thickness of the sedimentary cover, and deep seismic data on the Moho boundary depth. Part of the deep seismic profiles were digitized from the relevant publications.
3. The gravitational effect of the sedimentary cover on the vertical gravity gradient is forward calculated by approximating the sedimentary cover by a set of tesseroids. This effect was excluded from the vertical topographically corrected gravity gradient field.
4. An inversion of the satellite gravity gradient field was carried out, based on which a preliminary assessment of the Moho depth in the study area was made using the method of P. Haas et al. [Haas, Ebbing, Szwillus, 2020].
5. A three-dimensional density model of the Earth's crust and upper mantle of Volgo–Uralia was built in the process of forward gravity modeling in IGMAS+ software.
6. The necessary data for geothermal modeling were collected, which includes temperature and heat flow on the Earth's surface, temperature at the lithosphere-asthenosphere (LAB) boundary.
7. The program code for Bayesian inversion of geothermal parameters [Lösing, Ebbing, Szwillus, 2020] has been supplemented with the addition of the possibility of calculating geothermal parameters for a crustal model with multiple layers.
8. A statistical analysis of the geothermal structure of Volgo–Uralia was carried out using the previously obtained model of the lithosphere and the available data on the thermal field of the region under study.
9. Statistical differences in the structure of the Earth's crust and upper mantle and the values of thermal parameters within Volgo–Uralia were considered between two regions: (1) with existing hydrocarbon fields and (2) without discovered hydrocarbon fields.
10. Main directions for further work on the study of the crustal thermal properties and the analysis of the oil and gas potential of the Volgo-Uralian segment of the EEC have been determined.

Acknowledgements.

The author expresses his heartfelt gratitude to the scientific supervisor and the ideological inspirer of the study – Professor, Doctor of geological and mineralogical sciences Danis Karlovich Nurgaliev for useful discussions on the topic of the dissertation and comprehensive assistance and support at all stages of work.

The author expresses special gratitude to Prof. Dr. Jörg Ebbing and his colleagues Peter Haas and Mareen Lösing from the Christian Albrecht University of Kiel for the joint work, valuable comments and recommendations both in the process of performing the work itself and in the process of publishing the results of the study.

Special thanks to G.S. Khamidullina, N.N. Ravilova, Z.M. Slepak, D.I. Khasanov, E.V. Utemov, E.A. Yachmeneva, E.R. Ziganshin, P.S. Krylov and the entire staff of the Department of Geophysics and Geoinformation Technologies of the Institute of Geology and Oil and Gas Technologies of the

Kazan (Volga Region) Federal University for their support in writing, designing, and correcting the dissertation.

MAIN CONTENT OF THE WORK

The **introduction** substantiates the relevance of the research topic, formulates its purpose and objectives, as well as the scientific novelty and practical significance of its results, provides information about the approbation of the work and publications. Protected provisions are also presented here and the structure of the work is briefly characterized.

Chapter 1. Modern knowledge about the structure of the Earth's crust and upper mantle and its relationship with the thermal regime and hydrocarbon potential

Section 1.1 describes the current understanding of the structure of the Earth's crust and upper mantle and methods for its study. Definitions of the concepts of thermal lithosphere and craton are given. Seismic and non-seismic methods for studying the structure of the Earth's crust and upper mantle are considered. The method of gravimetry for studying the structure of the Earth's crust and upper mantle is considered in detail. Examples of models of the Earth's crust constructed using various approaches to working with the gravitational field are given.

In Section 1.2 the question of the relationship between the crustal structure and oil and gas content is considered. The thermal regime is highlighted as the main factor through which the crustal structure affects the hydrocarbon potential of the region. The calculation of the temperature distribution in the Earth's crust is shown and the factors leading to variations in the heat flow on the Earth's surface are listed. The relationship between the evolution of the crustal structure and the paleo heat flow in the course of the geological history of the formation of sedimentary basins is considered. Examples of the analysis of the thermal history of sedimentary basins are given and indicators of thermal maturity are considered.

The question of the direct influence of the crustal structure on the oil and gas content of the sedimentary cover is also touched upon. Specifically, the influence of crystalline basement fault-block structure on the hydrocarbon fields distribution is described.

Chapter 2. Object of study – Volgo–Uralia

Section 2.1 describes the tectonic structure and evolution of Volgo–Uralia as part of the East European craton. The structure of its crystalline basement and sedimentary cover is described. The evolution of the Earth's crust of Volgo–Uralia in the Precambrian and the formation of the structure of its sedimentary cover from the Paleozoic to the present time are considered.

Section 2.2 presents current data on the structure of the Volgo–Uralian crust, obtained mainly through seismic surveys.

Section 2.3 considers geothermal studies carried out on the territory of Volgo–Uralia throughout the history of its research. The modern understanding of the region's crustal thermal parameters variations is shown.

Chapter 3. Methodology for studying the crustal structure and the thermal regime of Volgo–Uralia

Section 3.1 provides input data and describes a gravity modeling technique for building a model of the Earth's crust and upper mantle of the Volgo–Uralian subcraton. The essence of the method consists in two main stages:

1. Inversion of the gravity gradient field with a laterally changing crust-mantle density contrast by using the Gauss-Newton algorithm with second-order Tikhonov regularization based on GOCE satellite data in order to preliminary estimate the depth of the Moho boundary within the studied region. Before the inversion, the gravity gradient field was corrected for topography and sedimentary cover. During the inversion, the value of the density contrast could change only between given tectonic

regions. Within the tectonic regions themselves, density contrasts remained unchanged. Four tectonic regions were selected for analysis: (1) Archean cratons, which included Volgo–Uralia, Sarmatia, and Fennoscandia, (2) Proterozoic rift belts, which included the Central Russia rift system, the Pachelma rift, the Mezen rift, and the Kama-Belsk rift, (3) Uralides, and (4) Precaspian Basin. A possible range of density contrast was determined: from 350 to 550 kg/m^3.

2. Forward gravity modeling in IGMAS+ software. Here, the map of the Moho depth obtained from the results of the gravity inversion was used as a preliminary model. The boundaries of the bottom of the sedimentary cover, the bottom of the upper crust, and the top of the asthenosphere were also added. Along with the structural information, the measured vertical gravity gradient field at the GOCE satellite flight altitude corrected for topography, the XGM 2019e Bouguer gravity anomaly at the Earth's surface, and seismic data on the depth of the Moho boundary were also imported. Further, the model of the Earth's crust of Volgo–Uralia was modified in such a way as to obtain a minimum misfit with the available measured gravity and seismic data.

Section 3.2 provides input data and describes the methodology for modeling the thermal field of the Earth's crust and upper mantle of the Volgo-Uralian subcraton. The essence of the method is the Bayesian Markov Chain Monte Carlo inversion based on surface heat flow and temperature data, as well as information on the structure of the Earth's crust and upper mantle of Volgo–Uralia, obtained in the process of gravity modeling.

Two models are considered: (1) single-layer crustal model with vertically constant radiogenic heat production and thermal conductivity and (2) multi-layer crustal model, consisting of three layers, sedimentary cover, upper and lower crystalline crust, also having vertically constant radiogenic heat production and thermal conductivity. Equations are derived for calculating the geotherms of the Earth's crust and upper mantle in stable cratonic regions for the single-layer and multi-layer models of the Earth's crust. Possible ranges of the analyzed thermal parameters variations for single-layer and multi-layer models of the Earth's crust are given.

Chapter 4. The results of the study of the crustal structure and the thermal regime of Volgo–Uralia and their relationship with hydrocarbon potential

Section 4.1 is devoted to the results of gravity modeling of the Volgo–Uralian crustal structure, which include the results of gravity inversion and forward gravity modeling.

As a result of the gravity inversion, the maps of the density contrast distribution between the Earth's crust and mantle, and a map of a preliminary estimate of the Moho depth within the studied region were obtained (Figure 1). The Moho reference depth during the inversion was 45 km. The density contrast between the Earth's crust and the upper mantle of the Archean cratonic crust and the Ural orogen was taken as 550 kg/m^3, while for the Paleoproterozoic rift systems and the Precaspian Basin it was taken as 500 and 350 kg/m^3, respectively. Such values are generally consistent with the study of the supposed crust-mantle density contrast according to the GOCE satellite data by M. Eshagh et al., which shows that it should be in the range of 400–600 kg/m^3 on the territory of Eurasia. [Eshagh and al ., 2016] The map of the Moho depth obtained as a result of gravity inversion is generally consistent with the known structural features of the Earth's crust in the region: the Earth's crust thickens in cratons and Uralides and thins along the Paleoproterozoic rifts, Cis-Ural trough, and the Precaspian sedimentary basin.

Forward gravity modeling in IGMAS+ led to the construction of a 3-D model lithospheric model of Volgo–Uralia (Figure 2). The model built in IGMAS+ has a standard deviation of the measured and calculated gravity fields equal to 8.0 mGal with a correlation coefficient between them equal to 0.91. For the vertical gravity gradient, the standard deviation was 0.13 etvos and the correlation coefficient was 0.81. In the process of model modification, an area with a significant discrepancy between the measured and calculated gravity fields reaching 95 mGal was found in the central part of Volgo–Uralia. This area was interpreted and modeled as a high-dense body at the base of the Vetluga synform which is confirmed by isostatic calculations. This conclusion is consistent with the previously proposed hypothesis of underplating in the center of Volgo–Uralia [Thybo, Artemieva, 2013] .

The constructed crustal model of Volgo–Uralia (Figure 3) shows the thickening of the Earth's crust in the craton areas up to 44–46 km compared to 40–42 km in the Paleoproterozoic rift belts that cut through the cratons. At the same time, within the area underplating in the center of Volgo–Uralia, the thickness of the Earth's crust exceeds 50 km, which is similar with that in the Ural Mountains (Figure 4). Significant thinning of the Earth's crust down to 32 km is observed in the Precaspian Basin and down to 34–36 km in the Cis-Ural foredeep, which is isostatically associated with thick sedimentary strata. Comparison of the constructed model with existing models of the Earth's crust showed that the developed model is closer to models created using seismic data (CRUST 1.0 and EUNAseis) than to a purely gravity GEMMA model. This fact speaks in favor of using seismic information about the depth of the Moho boundary to control the modelling of the Earth's crust based on satellite gravity data.

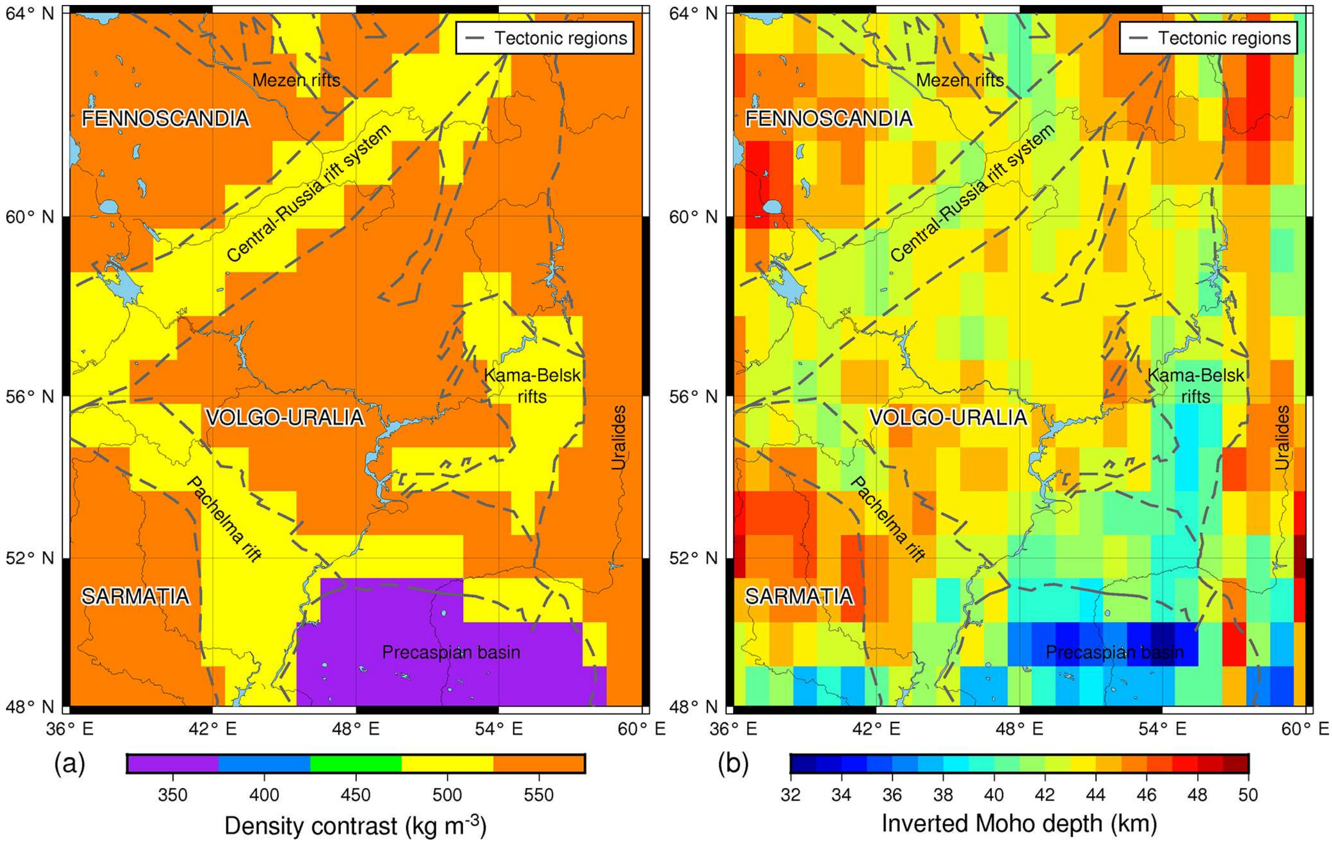

Figure 1. (a) Density contrast determined using the algorithm of Haas et al. [Haas, Ebbing, Szwillus, 2020] and (b) Moho depth obtained using gravity gradient field inversion

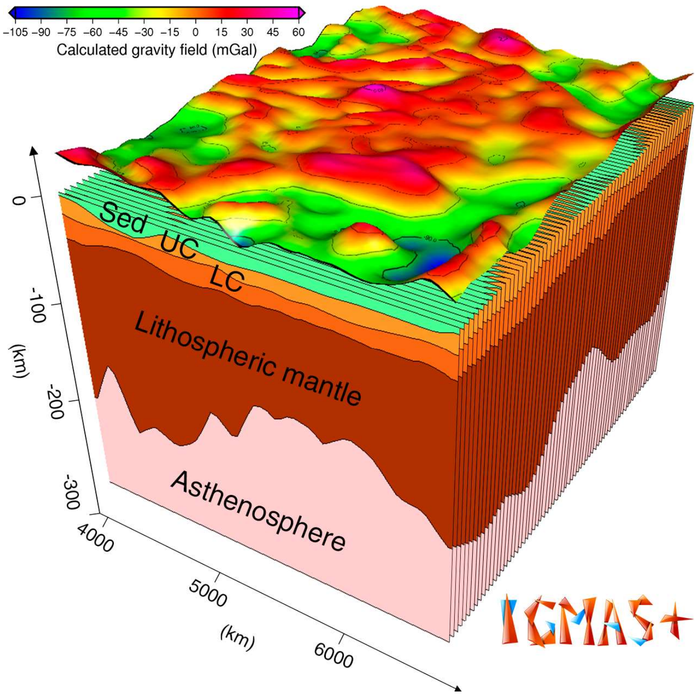

Figure 2. Three-dimensional model of the Volga–Uralian lithosphere built in the IGMAS+

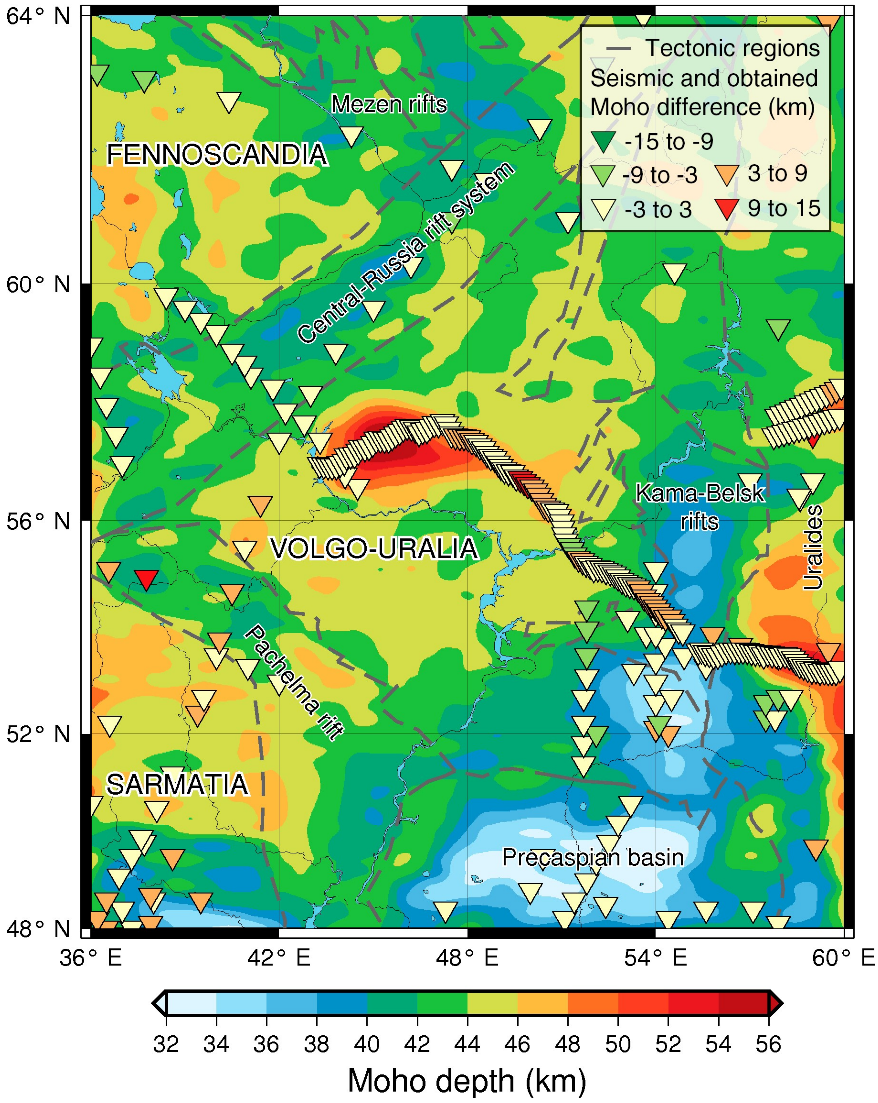

Figure 3. Moho model of the Volgo-Uralian subcraton obtained as a result of gravity inversion with laterally changing density contrasts and subsequent 3-D forward gravity modeling in IGMAS+

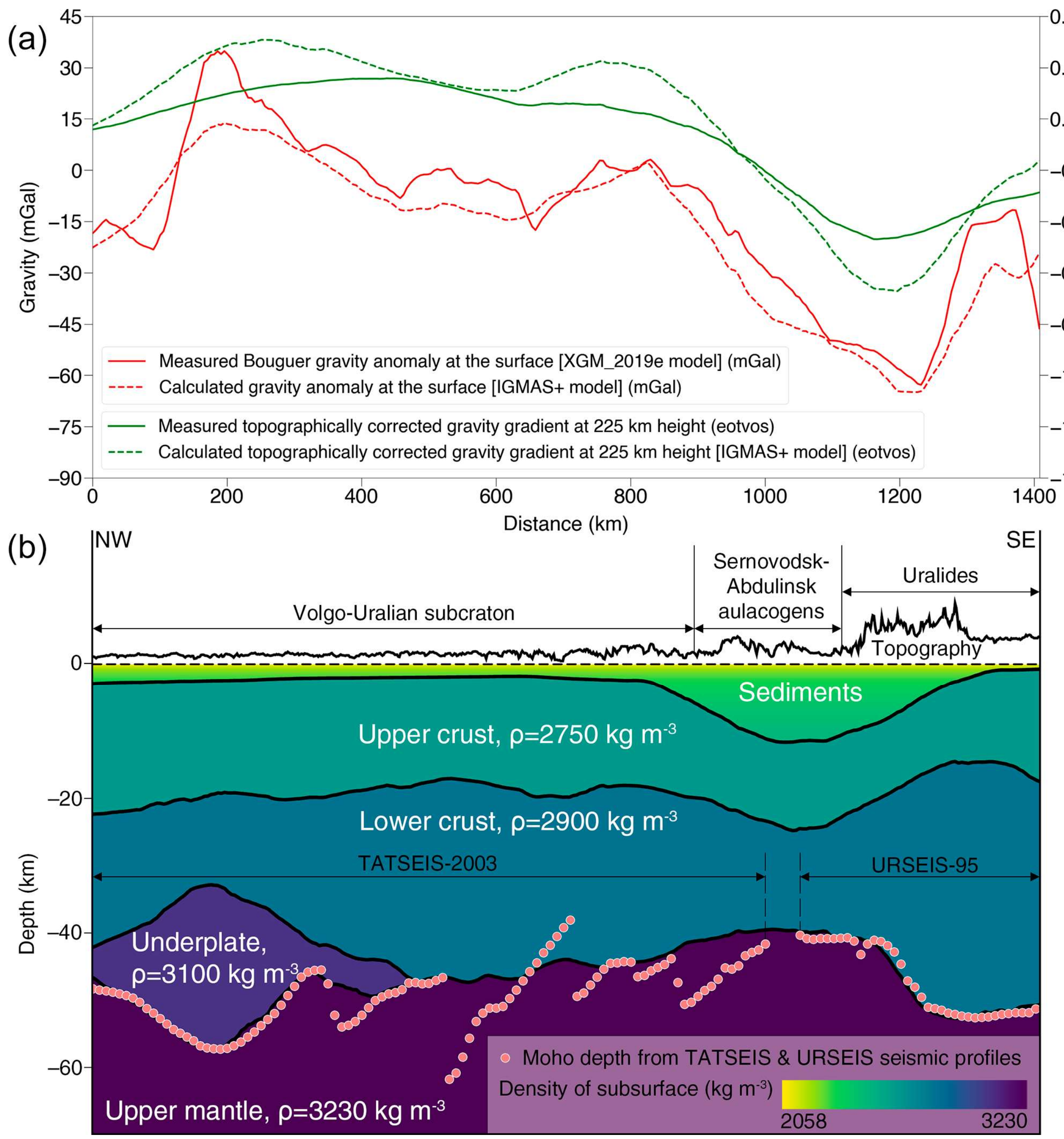

Figure 4. (a) Measured and calculated Bouguer gravity anomalies at the Earth's surface and topographically corrected vertical gravity gradient anomalies at GOCE satellite flight altitude. (b) Section of the IGMAS+ model along the TATSEIS-2003 and URSEIS-95 depth profiles

Section 4.2 is devoted to the results of geothermal modeling. Here the variations of the crustal and upper mantle thermal parameters of Volgo–Uralia found using Bayesian inversion for single-layer and multi-layer crustal models are described. The obtained maps of thermal parameters' variations for the single-layer and multi-layer models were calculated as the arithmetic mean of the last 90% of the solutions obtained by the Markov Chain Monte Carlo methods. The total number of solutions is 100000.

As a result, for the single-layer crustal model, significant variations in the RHP of the Earth's crust and mantle heat flow are observed. Variations of the crustal and mantle thermal conductivity are less pronounced (Figure 5). Thus, the average value of the crustal thermal conductivity for the study area was 2.06 W/m/K with a standard deviation of 0.27 W/m/K, while the mantle thermal conductivity has an average value of 3.74 W/m/K and a standard deviation of 0.14 W/m/K. Such a difference in the average values of thermal conductivities and their spread is due to different ranges set for this property. While the mantle thermal conductivity is almost uniform with minimal lateral variations in its values, the crustal thermal conductivity shows anomalies with low thermal conductivity of ~1.5–2.0 W/m/K in the Ural Mountains and eastern Fennoscandia, probably related to the features composition of crystalline rocks of these areas.

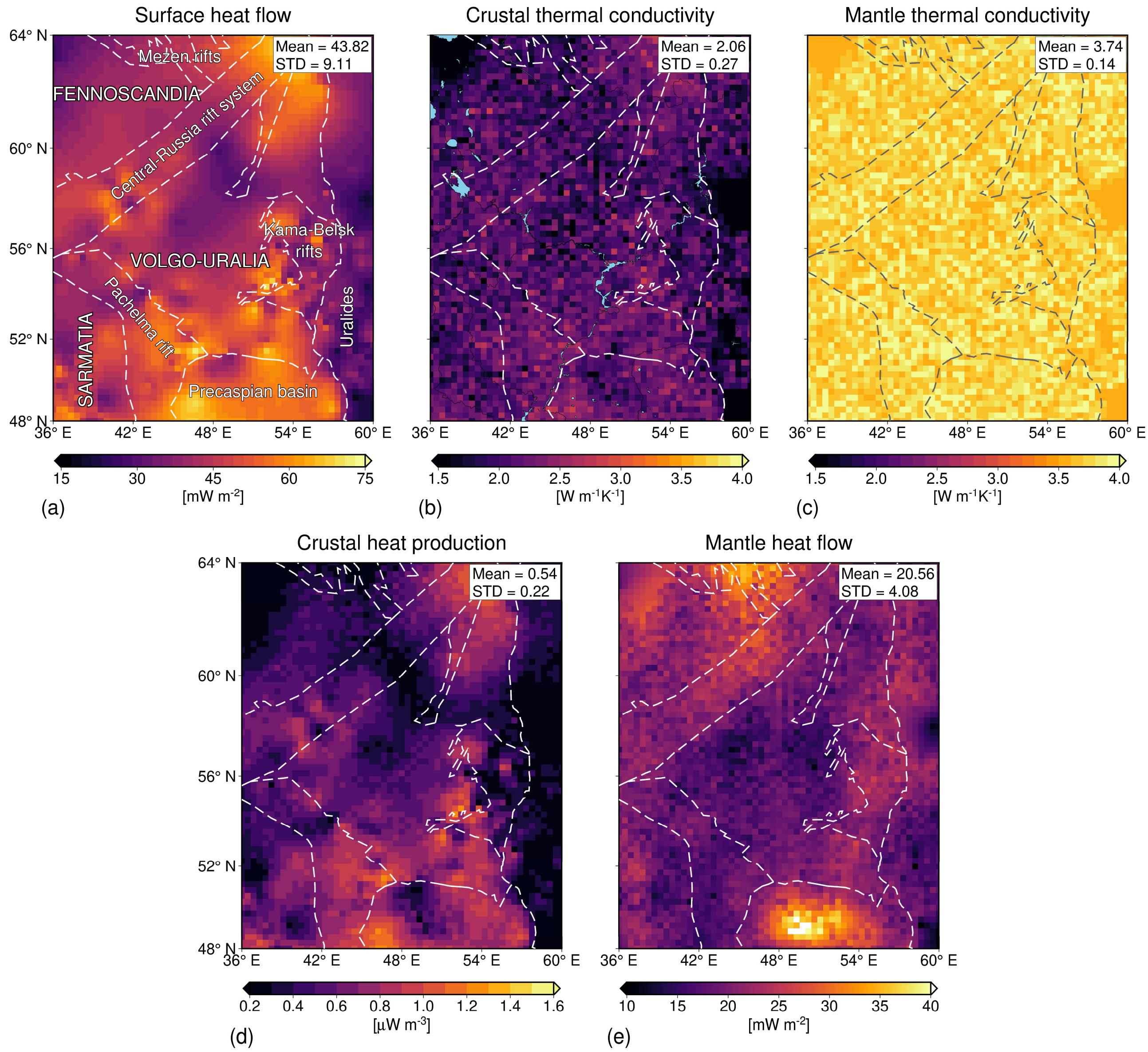

Figure 5. Variations in the thermal parameters of the Volgo-Uralian subcraton for the single-layer crustal model: (a) heat flow on the Earth's surface, (b) thermal conductivity of the Earth's crust, (c) thermal conductivity of the mantle, (d) RHP of the Earth's crust, (e) mantle heat flow

RHP of the Earth’s crust in the parameter which has much greater variation than thermal conductivity. It shows a low average value for the modeled region, equal to 0.54 μW/m^3. There are three regions with elevated RHPs: (1) the eastern part of Volgo–Uralia, (2) the south of Volgo–Uralia, the Precaspian basin and the Pachelma rift, (3) the Timan-Pechora basin in the north of Volgo–Uralia. There are also three regions with a reduced RHP: (1) the Ural Mountains, (2) Fennoscandia, and (3) the central Volgo–Uralia. Variations in RHP are primarily explained by variations in the composition of the crystalline crust. The mantle heat flow for the study region is also low, with an average value of 20.56 mW/m^2. An increase in the mantle heat flow to 30–40 mW/m^2 is observed in the region of the Precaspian Basin and Mezen rifts, a decrease to 10–15 mW/m^2 is observed in the region of the central Volgo–Uralia and the Ural Mountains. The anomalies of the mantle heat flow can mainly be explained by variations in the thickness of the thermal lithosphere, which is confirmed by the performed correlation analysis (Figure 6). From this analysis it also follows that the main parameter responsible for variations in the surface heat flow is the crustal RHP.

The multi-layer crustal model shows similar variations in thermal parameters with almost identical weighted averages of the thermal conductivity and crustal RHP to those of the single layer model. Correlations also practically do not change. Both models were tested using independent temperature measurements in boreholes and a temperature map at a depth of 1000 m in the Volga region [Kristoforova, 2002; Khristoforova et al., 2004] . As a result, a somewhat lower fit to the measured data was found for the multi-layer model. The results obtained allow us to conclude that the single-layer crustal model with constant RHP and thermal conductivity is a sufficient approximation for regional geothermal modeling.

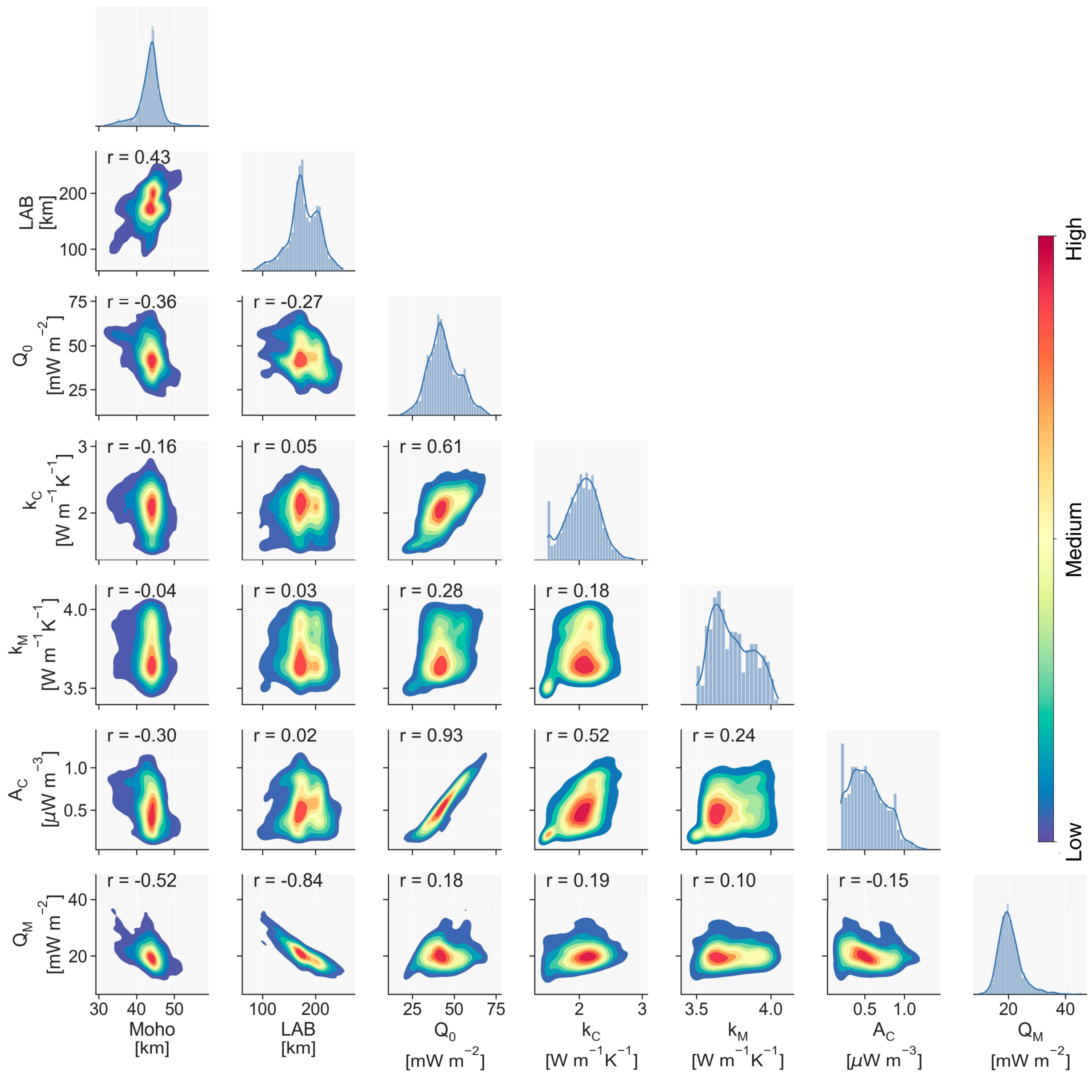

Figure 6. Correlogram of structural (Moho and LAB depths) and thermal parameters (heat flow on the Earth's surface Q_0, crustal RHP A_C, crustal thermal conductivity k_C, mantle thermal conductivity k_M, mantle heat flow Q_M) for the single-layer crustal model

In Section 4.3 the connection between the crustal structure and the hydrocarbon potential of Volgo–Uralia is analyzed. Based on the obtained maps of thermal parameters variations, a three-dimensional geothermal model of the Volgo–Uralian sedimentary cover was built. As can be seen in Figure 7, the thermal field of the Volgo–Uralian sedimentary cover is quite heterogeneous. Within the Volgo-Uralian subcraton, there is a relative increase in temperatures under the oil fields of the Volga-Ural hydrocarbon bearing province. This increase may be due to increased crustal RHP in this area.

The simulated increase in the crustal RHP in the southeastern part of Volgo–Uralia and the southern part of the Pachelma Rift reaches 1.2–1.4 μW/m^3 as compared to ~0.6 μW/m^3 in the cratonic part of Volgo–Uralia. Such an increase may be associated with the distribution of high-aluminous metasedimentary shales in these regions (Figure 8).

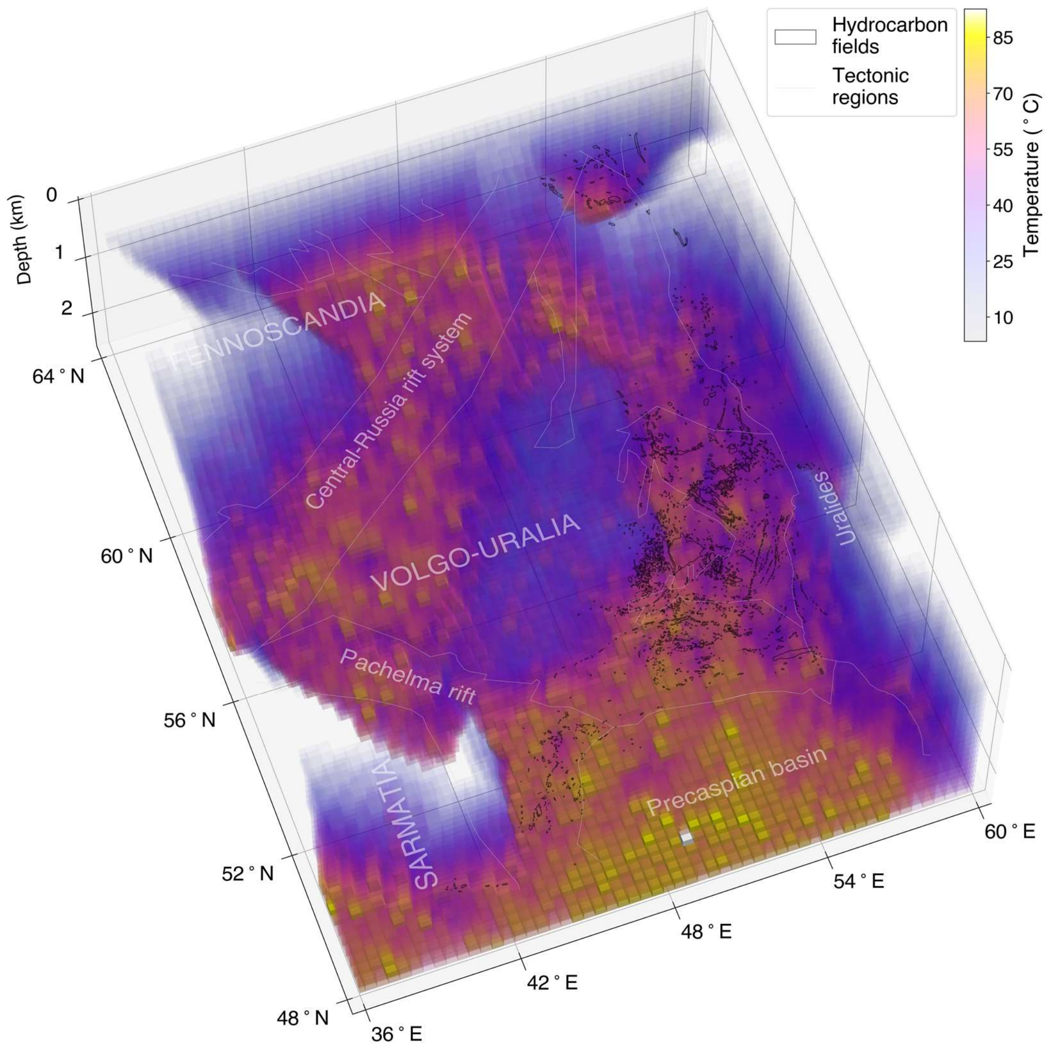

Figure 7. Three-dimensional voxel temperature model of Volgo–Uralian sedimentary cover

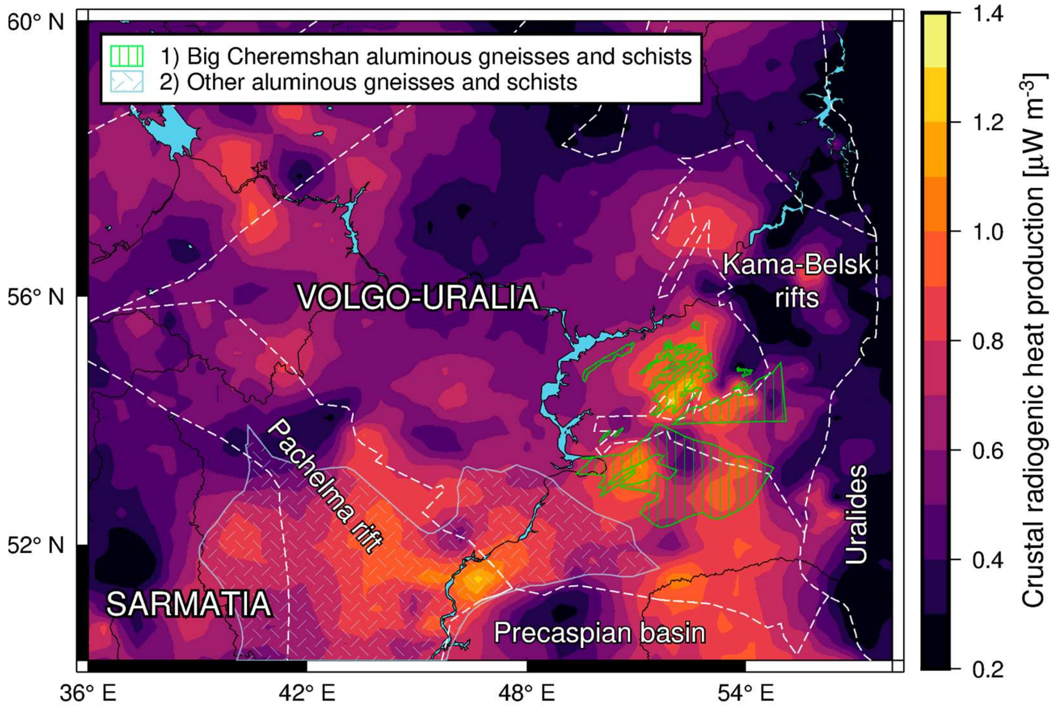

Figure 8. Radiogenic heat production in the southeast of Volgo–Uralia and its relationship with the distribution of metasedimentary complexes

The final step was to analyze the statistical significance of the difference between the simulated structural and thermal parameters within and outside the hydrocarbon fields of the Volgo–Uralian hydrocarbon bearing province (Table 1). Statistical analysis was carried out using Student's T-test for the difference in means with a significance level of 0.1%. As a result of the analysis, it turned out that the null hypothesis about the equality of mean values of the analyzed parameters cannot be rejected only for the mantle thermal conductivity. In the case of all other analyzed parameters, there is a statistically significant difference in their average values. The observed increase in crustal RHP, crustal thermal conductivity, and surface heat flow is probably associated with the changing composition of the crystalline crust in the Volga-Ural hydrocarbon bearing province, which contains metasedimentary high-aluminous shales of the Bolshecheremshanskaya series. An increase in the sedimentary cover thickness, a decrease in the thickness of the crystalline crust, and an increase in the mantle heat flow within the hydrocarbon fields are mainly associated with a decrease in the thickness of the thermal lithosphere.

Table 1- The main statistical characteristics of the studied parameters inside and outside the hydrocarbon fields of the Volga-Ural hydrocarbon bearing province

Parameter	Relation to HC fields	Median	Mean	STD	Dispersion
H_1 (km)	Inside	4.55	5.68	3.15	9.88
	Outside	2.83	4.33	3.08	9.46
H_2 (km)	Inside	15.79	15.56	2.58	6.65
	Outside	16.66	16.34	2.53	6.37
H_3 (km)	Inside	21.66	20.46	4.59	21.01
	Outside	24.07	22.83	4.57	20.85
M (km)	Inside	42.26	41.54	2.94	8.61
	Outside	43.88	43.33	2.47	6.08
LAB (km)	Inside	177.75	179.29	15.31	233.61
	Outside	183.95	190.8	24.09	579.17
k_C (W/m/K)	Inside	2.15	2.12	0.25	0.06
	Outside	2.07	2.06	0.26	0.07
k_M (W/m/K)	Inside	3.75	3.76	0.14	0.02
	Outside	3.71	3.73	0.13	0.02
A_C ($\mu W/m^3$)	Inside	0.66	0.62	0.25	0.06
	Outside	0.56	0.56	0.21	0.04
Q_M (mW/m^2)	Inside	20.3	20.42	2.32	5.38
	Outside	19.02	19.04	2.48	6.15
Q_0 (mW/m^2)	Inside	46.88	46.18	9	80.72
	Outside	42.28	43.03	8.18	66.77

Note: compiled by the author.

CONCLUSION

This study describes the modeling methodology and presents the crustal and geothermal models of the Volgo-Uralian subcraton. Based on the constructed models, an analysis of the relationship between hydrocarbon potential, the structure of the Earth's crust and upper mantle, and the thermal regime of Volgo–Uralia was performed.

The Volgo–Uralian crustal model was obtained using the inversion of the gravity gradient field and detailed object-oriented forward gravity modeling. The inversion of the gravity gradient field was performed using laterally changing density contrasts between the Earth's crust and upper mantle. Three different density contrasts were chosen: 350 kg/m^3 for the Precaspian sedimentary basin, 500 kg/m^3 for the Paleoproterozoic rifts, and 550 kg/m^3 for the Archean cratons and Uralides. The Moho reference depth was 45 km. As a result of the gravity inversion, a preliminary Moho depth map of Volgo–Uralia was obtained. Already at the stage of gravity inversion, the main patterns of the Earth's crust thickness undulations in the studied region were revealed. The model of the Moho boundary obtained by inversion of the gravity gradient field was further used as one of the density boundaries in the process of three-dimensional forward gravity modeling performed in the IGMAS+ software. Here, in addition to the Moho boundary obtained by gravity inversion, the following boundaries were added to the model: the bottom of the sedimentary cover, the bottom of the lower crust, LAB. The main data for tuning the model were seismic measurements of the Moho depth, the Bouguer gravity anomaly from the XGM2019e gravity field model, and the topographically corrected gravity gradient field from the GOCE satellite. Three-dimensional gravity modeling revealed a significant discrepancy between the measured and calculated gravity fields in the central part of the study area. This discrepancy was interpreted as an underplated body, which is confirmed by isostatic calculations and supports the hypothesis of an underplating located on the top of the Moho under the Oka block of Volgo–Uralia [Thybo, Artemieva, 2013].

The final model of the Earth's crust takes into account all the main geological features of the Volga–Uralian subcraton and its surroundings with the Moho thickening in the cratonic areas and under the Ural Mountains up to ~50–55 km and thinning along the Paleoproterozoic rifts, the Precaspian sedimentary basin and the Cis-Ural trough down to ~32–42 km. The resulting model of the Earth's crust served as the basis for further geothermal modeling.

The geothermal structure of Volgo–Uralia was studied by the Bayesian inversion using the MCMC method for two models of the Earth's crust: (1) single-layer crust and (2) multi-layer crust. The available geothermal and structural information was used to limit the possible solutions of the inversion, which resulted in the lateral variations in crustal and mantle thermal conductivities, crustal RHP, and mantle heat flow of Volgo–Uralia. The usage of multi-layer crustal model made it possible to study the distribution of thermal conductivities and RHP separately in the sedimentary cover, upper and lower crust. Although the average values of crustal thermal conductivity and RHP in the case of using the single-layer model differ from the average values of individual crustal layers for the multi-layer model, both models show similar patterns of thermal parameters' lateral changes, as well as their correlation trends.

Model validation against available temperature measurements did not show a significant improvement in convergence with temperature measurements when using the multi-layer model compared to the single-layer model. Therefore, it can be stated that the single-layer crustal model with constant RHP is a sufficient approximation for regional geothermal studies.

According to the single-layer model, the Volgo–Uralian crustal thermal conductivity remains almost constant with an average value of ~2.0–2.2 W/m/K in the study area with local decreases to ~1.5–2.0 W/m/K in the Uralides and the eastern Fennoscandia. The thermal conductivity of the sedimentary cover, the upper and lower crust in the multi-layer model have similar variations, while the thermal conductivity of sediments and the upper crust is higher compared to the thermal conductivity of the lower crust. The mantle thermal conductivity remains almost constant over the entire study area with an average value of ~3.75 W/m/K for the single-layer model of the Earth's crust and ~3.7 W/m/K for the multi-layer model.

Radiogenic heat production is the most important factor controlling the surface heat flow in the territory of Volgo–Uralia. Even though the sedimentary and upper crustal RHP of the multi-layer model is on average much higher than the bulk RHP of the single layer crustal model, the lower RHP of the lower crust compensates for this effect, giving nearly the same total crustal RHP in both models. As shown in the presented models, more than 50% of the total observed heat losses in the study area are accounted for by the RHP of the Earth's crust, which is consistent with the generally accepted opinion about crustal radiogenic heat production in the Precambrian regions (e.g. [Artemieva, Mooney, 2001]).

On a global scale, Volgo–Uralia is a region with low radiogenic heat production, averaging ~0.6 $\mu W/m^3$ in its cratonic part. Local increases of the crustal RHP are observed near high-aluminous metasedimentary complexes in the southern and eastern parts of the subcraton, where the RHP reaches ~1.2–1.4 $\mu W/m^3$. This relationship can also be the main reason for the anomalously high surface heat flow near the oil-bearing complexes of the South Tatar arch. Considering the close values of the volumetric crustal RHP in the single-layer and multi-layer models, the mantle heat flow remains practically unchanged in both cases. Variations in the mantle heat flow are mainly related to the thickness of the thermal lithosphere. Areas of thin thermal lithosphere, such as the Mezen rifts in the east of Fennoscandia and the Precaspian sedimentary basin on the south of the study area, have an increased mantle heat flow reaching ~30–40 mW/m^2. The central Volgo–Uralia is characterized by a low mantle heat flow with values of ~15–20 mW/m^2.

The statistical analysis of the relationship between the structure of the Earth's crust and the upper mantle and variations in their thermal parameters showed that the sedimentary cover thickness, the thickness of the upper and lower crust, the Moho depth, the LAB depth, the crustal thermal conductivity and RHP, the mantle and surface heat flow have a statistically significant difference in average values inside and outside the existing hydrocarbon fields within the Volga-Ural hydrocarbon bearing province. These differences are explained both by the structural and tectonic features of the Volgo–Uralia, and by the heterogeneity of the composition of its crystalline basement. The only exception is the mantle thermal conductivity, for which no statistically significant difference in the mean values was found.

The obtained structural and geothermal models can serve as a basis for further basin analysis of the Volga-Ural region, which, together with geochemical data, can more accurately reveal the processes of generation, migration, and accumulation of hydrocarbons in the Volga-Ural hydrocarbon bearing province. Additionally, it is recommended to conduct studies on the radiogenic heat production variations of crystalline rocks of the Otradnenskaya and Bolshecheremshanskaya series, as well as other metasedimentary rocks of Volgo–Uralia. Such studies can verify the conclusions drawn in this dissertation about radiogenic heat production as the main factor controlling the surface heat flow of the Volga-Ural region.

THE MAIN SCIENTIFIC RESULTS OF THE RESEARCH ARE REFLECTED IN THE FOLLOWING PUBLICATIONS OF THE AUTHOR:

1. The thermal state of Volgo–Uralia from Bayesian inversion of surface heat flow and temperature / I. Ognev, J. Ebbing, M. Lösing, D. Nurgaliev // Geophysical Journal International. 2023 Vol. 232, Issue 1, pp. 322–342. (1.3 / auth. 0.3 p. l.)
2. Ognev I. Crustal structure of the Volgo–Uralian subcraton revealed by inverse and forward gravity modeling / I. Ognev, J. Ebbing, R . Haas // Solid Earth. 2022 Vol. 13, Issue 2, pp. 431–448. (1.1 / auth. 0.4 p. l.)
3. Ognev I.N. Interrelation between the structure of the Earth's crust and upper mantle and the maturity of source rocks / IN Ognev, DK Nourgaliev // GEOMODEL 2019 – 21st Conference on Oil and Gas Geological Exploration and Development. European Association of Geoscientists and Engineers, EAGE, 2019. Vol. 2019. Code 160681 (p. 1–5). (0.3 / auth. 0.15 p. l.)
4. Ognev I.N. The use of "native" wavelet transform for determining lateral density variation of the Volgo–Uralian subcraton / IN Ognev, EV Utemov, DK Nurgaliev // SOCAR Proceedings. Oil Gas Scientific Research Project Institute, 2021. Vol. 2021, Special Issue 2, pp. 135–140. (0.4 / auth. 0.1 p.l.)
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7. An example of the reconstruction of the processes of accumulation of carbonate sediments based on seismostratigraphic and paleogeomorphological analyzes / B. V. Platov , G. S. Khamidullina , I. A. Nuriev , I. P. Novikov , I. N. Ognev // Oil Industry. 2018. No. 1. P. 18–22. (0.3 / auth. 0.06 p. l.)