The thesis document includes the following changes in answer to the external review process.

Dear Jury Members,

I express my gratitude for your valuable comments and suggestions. I found all of them highly important since they resulted in a significant improvement of the thesis quality. I carefully addressed all issues and answered below, point-by-point, with your comments in italic.

Reviewer Prof. Massimo Verdoya:

All in all, the text is a bit wordy, with several repetitions. Some sentences would be clearer if shortened. Even if I am not a native English, I found some evident grammar and spelling errors that may cause misleading interpretations and confusion in the text. Thus, I annotated the PDF with my comments and suggestions that I recommend incorporating in the final version.

Response: Thank you for the thorough revision of the thesis that allowed me significantly increasing the text quality. I accepted all your text correction recommendations and provided answers to several comments that required my responses below, point-by-point. Please, see them.

- Page 27: This is unclear. How can one produce a well-log approach if logging tools are unavailable? I suggest revision of this sentence.
  Response: Thank you for the comment. I removed this part of the sentence.

  Response: Thank you for the comment. I meant the regression model-based approach. I revised the sentence the following way: “Therefore, the application of regression model-based approach might be challenging in the case of low porosity and low contrast of physical properties in the rock components”.

- Page 31: Unclear: do you mean that there are too few applications of machine learning techniques to this problem?
  Response: Thank you for the comment. Yes, I meant that there are only a few examples of machine learning technique implementation. I revised the sentence the following way: “Lack of implementations of machine learning techniques for problem solution”.

Response: Thank you for the comment. I revised the sentence the following way: “Moreover, without reliable data on rock thermal properties, largely different scenarios for organic matter maturation may result from basin and petroleum system modelling affecting results of assessment of hydrocarbon potential for a given region (Chekhonin et al., 2019)”.

- Page 34: Delete “incomparable in terms of spatial resolution”. “Neglecting differences in the vertical resolution of analyzing data in case of heterogeneous rocks obviously leads to unreliable results” - This concept has been already stated before. Repetition. I suggest deletion.

Response: Thank you for the comment. I believe that deleting this part results in the disconnection of the subsequent part of the section with the beginning part. I wanted to emphasize one more time the problem to illustrate after that the example of consequences when heterogeneity is neglected. Thus, I left this part in the revised text. Hope to get your understanding.

- Page 37: *what do you mean with high productivity? Unclear.*

Response: Thank you for the comment. For high productivity, I mean that we can conduct measurements on numerous core samples during a short period of time. I substituted “high productivity” to “high rate”.

- Page 42: *simple?*

Response: Thank you for the comment. I mean universally applicable. I revised the sentence the following way: “Hence, there are no universally applicable correlations that can be used for predicting rock thermal properties”.

- Page 46: *Unclear sentence. It is not clear what you mean with azimuthal and transversely isotropic. Could you simplify the description?*

Response: Thank you for the comment. I revised the sentence the following way: “According to Chekhonin et al. (2018) the Bazhenov Formation in the investigating region is characterized by negligible 3D thermal anisotropy (that was assessed on flat ends of full-size core samples) and can, therefore, be treated as a transversely isotropic medium (2D anisotropy) with the vertical axis of symmetry.”

- Page 47: *Did I miss anything? The B. F. above is defined with "negligible azimuthal anisotropy" and "transversely isotropic", whereas here is "highly anisotropic". Could you explain better?*

Response: Thank you for the comment. The Bazhenov Formation exhibits 2D anisotropy. I mentioned this in the above sentence. Please, see it.

- Page 48: *How do you infer it? Give a brief explanation or reference.*

Response: Thank you for the comment. I added the reference to Balushkina et al. (2014).

- Page 54: *Unclear. Reformulate the sentence.*

Response: Thank you for the comment. I revised the sentence the following way: “Extending the approach described in Section 2.1 for predicting rock thermal properties from sonic log data we involve additional logs and multiple regression analysis for predictions. The assessment of the effectiveness of diverse machine learning methods for determining rock thermal properties was performed.”

- Page 63: *Sentence long and unclear.*

Response: Thank you for the comment. I revised the sentence in the following way: “The novel approach described in Section 2.1.1 for predicting rock thermal properties from sonic log data was extended by involving additional logs and multiple regression analysis using machine learning. The assessment of the effectiveness of diverse machine learning methods for determining rock thermal properties was performed.”
Page 70: Do you mean that accurate logs (sonic, density and neutron) are more important to correctly predict thermal properties?

Response: Thank you for the question. I mean that the presence of these logs in the logging suite enables precise predictions of rock thermal properties. I revised the paragraph in the following way: "The sensitivity study of regression models of gradient boosting algorithm for predicting rock thermal properties was conducted using the input perturbations method. The obtained results revealed that so-called porosity log data (sonic, density and neutron log) have the highest relative importance for predicting rock thermal properties."

Page 103: Unclear. Is it SiO2?

Response: Thank you for the question. Yes, the siliceous component that consists mainly of silicon dioxide, either as quartz or as amorphous silica.

Page 123: This part of the text is unclear. One cannot call apart what is novel (that is partly presented in this thesis) and what is taken from previous studies. I suggest revision and shortening to clarify it.

Response: Thank you for the question. I revised the sentences the following way: “In this Chapter we present two case studies of geothermal investigations of prospecting and appraisal wells located in Russia. The performed investigations were conducted by means of the modern methodological and experimental basis of thermal petrophysics. The performed geothermal investigations demonstrated that the WLBT for determining rock thermal properties is a critical component for reliable determining vertical variations of heat flow density.”

Page 123: Is it necessary to introduce a subsection here?

Response: Thank you for the question. I believe that it is necessary here. It makes the text of the Chapter more structured.

Page 123: Why did you use 80% and 20% of data instead of the same subdivision (66-34%) used for the over case studies?

Response: Thank you for the question. During regression model training, we found that subdividing dataset into 66 and 34% subsets resulted in overtraining the gradient boosting. We assume that this can be due to the data size. After several iterations, we found that subdivision into 80 and 20% stabilize the learning process.

Page 123: Is the T measurement spacing 10 cm? Clarify. Could you provide details (type of sensor, precision) on the equipment used for T measurements?

Response: Thank you for the comment. Yes, the spacing during temperature logging was 10 cm in both wells. Unfortunately, we do not have an access to information about sensor type that was used during measurements in the investigated wells as the measurements were performed by our industrial partner as I mentioned in the thesis after the correction (please, see pages 127 and 140). However, we assume that a thermistor was used as the temperature sensor. Following the ISRM recommendations (see, Popov et al., 2016, doi: 10.1007/s00603-016-1070-5) for precision I understand the random error during temperature measurements. The precision of temperature measurements in our cases did not exceed ±0.007 °C (at 0.95 confidence level) according to the instrument certificate. It is sufficient for the measurement quality characterization in our case. I added the information about measurement precision in the revised thesis (please, see pages 127 and 140). I should also note that we recently developed the approach for assessing the precision of the temperature measurements in wells (during temperature logging) to characterize the uncertainty in data on temperature gradient that is required for registering detailed vertical variations in heat flow within short depth intervals (from 3 m and larger).

Page 159: Change title “Summary and Conclusions” to “Concluding remarks”
Response: Thank you for the question. According to the official recommendations of Skoltech, the last part of the thesis should be “Summary and Conclusions”. To follow the recommendations, I did not change the title. Hope to get your understanding.

While revising the text I suggest also consider the revision of the titles of the chapter sections and subsections. I found that they are very wordy, and this again causes confusion in the reader. I suggest shorter and synthetic titles. This also will reverberate in the thesis index, which in my opinion, should give at a glance of the logical sequence of the work.

Response: Thank you for revision of the titles. I accepted all your recommendations. Please, see the revised version of the thesis.

Finally, I also suggest the addition of some figures illustrating the location of the case history boreholes/investigated areas. In case this is not possible for this information is confidential, I suggest at least a sketch of the geology/geography surrounding the borehole/s. A reader can be rather confused by the several formation names and sites without at least a rough geological/geographical information.

Response: Thank you for the suggestion. I added the location of the wells (please, see pages 124 and 138 in the revised thesis).

Reviewer Prof. Shaopeng Huang:

Comments:

1. **Table 1.** I don’t understand why the sum of the mean mass contents exceed far beyond 100%.

Response: Thank you for the comment. As I mentioned below the Table 1, at each specific depth point, the sum of mineral content, organic matter, and porosity at each specific depth point yields 100%. The Table contains the mean mass content of each mineral along the investigated geological profiles for two formations (the Bahzenov and the Domanic). Thus, the sum of mean mass contents should not yield 100%.

2. **Table 2.** The parallel thermal conductivity measurements are systematically greater than the vertical ones. The thesis attributes the difference to the orientation of organic matters in the sample. However, could it be possible that the difference could be caused by the fact that the parallel conductivity is measured on the surface while the vertical conductivity is measured on the flat surface of the core? Please, add some discussions to exclude this possibility if you think there is a technical bias here.

Response: Thank you for the comment. All involved experimental data was obtained on the same flat surface of core samples. The thermal conductivity both for parallel and perpendicular directions to the bedding plane was measured on the same flat surface of the sawed full-sized cores (Figure 1). Thus, the thermal anisotropy is not caused due to some technical reasons.

A common reason (except specific organic matter distribution) leading to thermal anisotropy is the micro fracturing (that occurs during sedimentation or due to unloading of core samples after recovery) that in most cases has parallel to the bedding plane orientation and that decreases the perpendicular to the bedding plane thermal conductivity (please, see Popov et al., 2016, doi:10.1007/s00603-016-1070-5).

3. **Table 3.** The Depths of investigation of the applied well-logging tools are in tens of centimetres?
Response: Thank you for the comment. The depth of investigation is presented in centimetres. There are no typos. I checked it in the logging tool specifications.

4. **There are some typos and subscripts/superscript need to be corrected.**

Response: Thank you for the comment. I performed several proofreadings with the help of my colleagues and essentially enhanced the language quality. Please, see the revised text.

**Reviewer: Dr. Irina Bayuk**

Comments:

1. The author of dissertation writes that the stiffness tensor can be simply estimated from the data provided by the dipole sonic tool. However, this is not always the case. It is only valid if two assumptions are met: (a) $C_{12} = C_{13}$ and (b) the Thomsen parameters delta is close to zero. These assumptions follow from observations on shales, not from the theory. However, in some cases these assumptions are failed. Therefore, it would be more correct to pay attention on these assumptions and verify them in laboratory experiment for rocks under study.

Response: Thank you for the comment. Of cause, the stiffness tensor cannot be simply estimated from the data provided by the dipole sonic tool. Not to confuse readers, I added the following comments about the constraints you mentioned:

“For the investigating wells, the results of cross-dipole sonic logging were available. From those results, sonic velocities for parallel and perpendicular to the bedding plane directions were inferred assuming that elastic constants $C_{12}$ and $C_{13}$ are equal and the Thomsen parameters delta is close to zero (see Schoenberg et al., 1996).” (please, see page 49).

I absolutely agree that these assumptions must be verified experimentally on the investigating rock samples from the Bazhenov Formation, which is quite exceptional in terms of its properties. I added your recommendation to “Recommendations” section as a subject for further investigation.

2. The author suggests to estimate the principal axes of symmetry using geomechanical experiment. However, these experiments are rather expansive. Besides, samples are destroyed after the experiments. It would be better to use for this purpose laboratory measurements of elastic wave velocities, specifically, multilevel ultrasonic sounding. This method allows one to discriminate between the anisotropy and heterogeneity and estimate the anisotropy type. Besides, this method is non-destructive.

Response: Thank you for the comment. Following your recommendation, I extended the part about determining principal axes of symmetry the following way: “… or through a multilevel ultrasonic sounding as described by Tikhotsky et al. (2018).” (please, see page 44).

3. **Figure 6. What do the solid and dashed grey lines mean?**

Response: Thank you for the comment. Solid line presents a perfect prediction of rock thermal properties ($x=y$), grey dashed lines present the prediction uncertainty intervals. I revised Figure 6 and the caption in the following way:
Figure 6. Results of prediction of thermal conductivity for parallel (left panel) and perpendicular (central panel) direction to the bedding plane from sonic velocity and rock volumetric heat capacity from photoelectric factor (right panel). Solid line presents a perfect prediction of rock thermal properties (x=y), grey dashed lines presents the prediction uncertainty intervals.

4. **Figure 6. For the VHC and PEF the correlation is very poor. Please, comments on this point.**

Response: Thank you for the comment. The correlation between PEF and volumetric heat capacity is of a lower quality (according to $R^2$) compared to thermal conductivity for the following reasons:

- The measurement quality of both photoelectric factor ($\pm 6\%$ according to technical specifications of the measuring tool) and volumetric heat capacity ($\pm 5\%$ for the field optical scanner during express measurements) cannot be considered as quite high (compared to measurements of thermal conductivity) considering the variation range of the volumetric heat capacity (from $1.7$ to $2.3 \, \text{MJ} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$ in the presented case) and photoelectric factor. That affects the quality of interrelation between volumetric heat capacity and photoelectric factor.
- Lower contrast between volumetric heat capacity of rock matrix and organic matter (compared to the contrast of thermal conductivity of matrix and organic matter). Based on results of our calculations, an approximate value of volumetric heat capacity of organic matter from the Bazhenov Formation is $1.61 \, \text{MJ} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$ (see, please, Shakirov et al., 2021, https://doi.org/10.1016/j.geothermics.2021.102059). Whereas, the volumetric heat capacity of rock-forming minerals varies from $1.85 \, \text{MJ} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$ to $2.40 \, \text{MJ} \cdot \text{m}^{-3} \cdot \text{K}^{-1}$.

Anyway, the established correlation coefficient is statistically significant according to Student t-test (for 0.95 confidential probability level) and therefore the established regression equation can be used for predictions.

5. **For theoretical modeling of anisotropic rocks several methods that include correction factors for directions parallel and perpendicular to the bedding are used. The choice of two correction factors was needed to incorporate the anisotropy in thermal conductivity observed in experiment. This means that two unknown values (correction factors) should be found to satisfy the experimental data. The author compared a quality of the thermal conductivity prediction based on (a) theoretical modeling based on the methods with correction factors and (b) regressions combined with machine learning. The author demonstrated that variant (a) produces worse results compared to (b). I advise to use EMT methods here for the theoretical prediction. These methods take into account anisotropy since give resulting thermal conductivity in a tensorial form. Besides, to incorporate anisotropy, only one correction factor is required instead of two – aspect ratio of oriented non-isometric inclusions. However, the author understand that more physically justified theoretical approaches should be used. Thus, this comment can be considered as an advice for the future work.**

Response: Thank you for the comment and advice for future work. I also added an extended discussion of the application of EMT methods to “Recommendations” section. Please, see it.

Another aspect that requires comprehensive investigations is determining the type of distribution function for orientation and shape of minerals, pores and fractures within unconventional reservoirs (such as the Domanic and the Bazhenov Formations). The vertical variations of the aspect ratio of oriented non-
isometric inclusions along the geological profiles of unconventional reservoirs is another issue to be studied. Anyway, the application of EMT methods (compared to so-called “mixing” rules) is more beneficial since they enable predicting no only thermal conductivity but other tensorial physical properties (such as sonic velocities and electrical resistivity) from knowledge on aspect ratio of oriented non-isometric inclusions and physical properties of rock matrix.

Reviewer: Prof. Ramil Sharafutdinov

Comments:

1. I can see that regression based approach in most cases yields more precise predictions compared to theoretical-model based. Please extend the discussion on the conditions when theoretical-model based approach is preferable.

Response: Thank you for the comment. I extended the discussion on conditions of application theoretical model-based approach the following way:

"Based on results presented in Figs. 11 and 12, we can conclude that the gradient boosting method is more effective for predicting rock thermal properties than the theoretical models because of its high sensitivity to the non-linear and implicit dependencies between the rock thermal properties and well-logging data. However, in case rocks are low porous or have low organic matter content the correlations between thermal and other physical properties can diminish and the quality of predictions will be unacceptable. Moreover, the application of gradient boosting requires training datasets, which are not always available. Therefore, for cases when core samples are absent and only well-logging data are available or the rocks are low porous (or which have low organic matter content), predictions of rock thermal properties can be performed with sufficient precision based on theoretical models. Another benefit of application of theoretical modelling approach is opportunity of transition from one saturation state to another. In case of lateral variations of rock saturation the regression model based approach requires determining corrections to rock thermal properties for different saturations on the basis of special experimental investigations (see, e.g., Popov et al., 2017) whereas the theoretical model based approach does not."

The added part is in italic. Please, see page 83.

2. Please, highlight the novelty of the obtained results in the abstract.

Response: Thank you for the comment. The novelty of the research results was highlighted in the following way:

"A new technique for the simultaneous determination of rock thermal conductivity and volumetric heat capacity from well-logging data accounting for thermal anisotropy, heterogeneity and in situ thermobaric conditions was developed and tested on vast representative experimental data from various hydrocarbon fields, including organic-rich shales and heavy oil field. The novelty of the technique includes integration of thermal core logging and well logging data and application of theoretical models and regression analysis via machine learning. The implementation of the novel well-log based technique for determining rock thermal properties within the geothermal investigations allowed obtaining new data on vertical variations of rock thermal properties and heat flow density that enhanced the quality of the subsequent studies of hydrocarbon fields."

Please, see the Abstract.

3. From the obtained results, I see that thermal conductivity perpendicular to the bedding plane cannot be predicted with the same quality as thermal conductivity parallel to the bedding plane. Please extend the discussion on that issue.

Response: Thank you for the comment. I extended the discussion on that issue the following way (please, see page 62):
“This can be due to the more significant influence on the thermal properties perpendicular to the bedding plane of micro-cracking from core unloading. Another reason is rock heterogeneity. Since during thermal core logging along the perpendicular directions to the bedding plane we conduct only several measurements on one core sample the obtaining values of thermal conductivity perpendicular to the bedding plane can be biased due to rock heterogeneity.”

4. I do not see any recommendation for future research. Please add.

Response: Thank you for the comment. I added the “Recommendation” section in the revised version of the thesis. Please, see it.

5. You presented a new data on terrestrial heat flow in the implementation part. If possible, please add the maps with well locations.

Response: Thank you for the suggestion. I added the location of the wells (please, see pages 124 and 138 in the revised thesis).

6. You addressed your research only to sedimentary rocks. Please add the discussion on applicability of your technique to other types of rocks.

Response: Thank you for the comment. I believe that the application of the developed technique is not tightly constrained to sedimentary rocks from the physical point of view. However, I did not have the experimental data for validation. Thus, I added the discussion on that issue in the “Recommendation” section as a possible part of future research. Please see it.

7. Please check once again for the grammatical typos. I have seen several of them within the text.

Response: Thank you for the comment. I performed several proofreadings with the help of my colleagues and essentially enhanced the language quality.

Reviewer Prof. Alexey Cheremisin:

Comments:

After thoroughly reading the text of the dissertation, I recommend finalizing the presented work in accordance with the following recommendations:

1. To compare the proposed methods for assessing the thermal properties of sedimentary rocks, indicating the comparison metrics and provide information in the conclusion section.

Response: Thank you for the comment. The comparison analysis of the theoretical model-based and the regression model-based analysis was presented in subsections 3.1.2 (see page 81) and in section 4.2 (please, see pages 102-117). I added the summary of comparison analysis in the “Summary and Conclusion” Section in the following way:

“From comparison of measured and predicted profiles of rock thermal properties it can be concluded that thermal conductivity for parallel and perpendicular direction to the bedding plane and volumetric heat capacity using the developed regression and theoretical model-based approaches can be predicted with uncertainties of less than 10%, 15%, 10% (for 0.95 confidential probability level), respectively. The regression model based approach in most cases yields more precise predictions of rock thermal properties compared to theoretical model based.”

Please, see bullet 3 on page 160.

2. Provide data on the division of authors’ contribution for works published as part of the dissertation work.

Response: Thank you for the comment. I added the author contributions after publication list. Please see page 6.

3. The thesis text contains multiple grammatical and syntactic errors; proofreading is required.
Response: Thank you for the comment. I performed several proofreadings with the help of my colleagues and essentially enhanced the language quality.

Reviewer: Prof. Dmitri Pissarenko

No corrections were requested.