



## Editorial A Summary of "Petrophysics and Geochemistry of Unconventional Reservoirs"

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Unconventional reservoirs are discovered in all petroleum basins around the world. Their exploration and production are an increasingly important challenge for the oil and gas industry due to maturation of conventional plays and depletion of conventional petroleum resources. The complexity of unconventional reservoirs' development is associated with significant uncertainties and risks, which lead to high production costs. Kerogen-rich rocks in unconventional reservoirs exhibit high heterogeneity on a wide range of scales, and their physical properties are typically highly anisotropic. Comprehensive petrophysical and geochemical studies are of particular importance in the analysis of petroleum generation and accumulation processes in unconventional plays. Studies of kerogen-rich rocks are of crucial importance for the development and optimization of production technologies, including hydraulic fracturing and various methods of enhanced hydrocarbon recovery. Consequently, a multidisciplinary approach for the evaluation of unconventional resources is essential for successful exploration and development projects. This Special Issue aims to reflect new ideas, concepts, and methods in research related to petrophysics, lithology, and geochemistry of unconventional formations, including but not limited to reservoir properties, mechanical and thermal properties, and molecular and isotope composition of organic matter, as well as the mechanisms of rock and organic matter transformations during geological history and hydrocarbon production.

Spasennykh et al. [1] present a study on geochemical trends reflecting hydrocarbon generation, migration, and accumulation in the Bazhenov shale rock formation of the central part of the West Siberian Basin (Russia). More than 3000 pyrolysis analyses were carried out for a representative sample collection containing rock samples with varying organic matter maturity from 34 wells, and the developed procedure includes analyses of samples before and after the extraction by organic solvent. Summarized results in the forms of cross-plots and diagrams reveal the quantitative trends in the changes of generation potential, amount, and composition of generated hydrocarbons in rocks at different stages of oil generation. The analysis of these trends allows specialists to improve approaches for productivity evaluation and study the effect of organic matter maturity on the distribution of productive intervals of different types for the Bazhenov formation.

During the last decade, the use of stable isotopes of bio (e.g., hydrogen, carbon, nitrogen, oxygen, sulfur) and trace (e.g., Sm, Nd) elements has become increasingly popular for petroleum exploration, not only in conventional but also in unconventional petroleum basins. Several papers in this Special Issue demonstrate how this approach can be used for investigating the depositional conditions and diagenetic processes during the formation of source rocks [2–4] as well as the mechanisms that accompany biodegradation of petroleum hydrocarbons [5].

Leushina et al. [2] report the results of geochemical studies and reconstruction of paleosedimentation conditions of Upper Jurassic–Lower Cretaceous source rocks from the north of Western Siberia (Russia). The rocks are characterized by significant variations in total organic carbon content and petroleum generation potential of organic matter; the maturity



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**Copyright:** © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). is at the beginning of the oil window. The authors integrate isotopic data with geochemical analyses to evaluate the genesis of the rocks in the peripheral part of the Bazhenov Sea and reconstruct paleoenvironments that controlled the accumulation of organic matter in sediments, its composition, and diagenetic alterations. According to the obtained data, the deposits of the Northern Bazhenov accumulated under marine conditions with a generally moderate and periodically increasing terrigenous influx. The variations in organic matter composition are determined by redox conditions and terrigenous input which correlate with the eustatic sea-level changes during transgressive/regressive cycles and activation of currents. Transgression is associated with an intensive accumulation of organic matter under anoxic to euxinic conditions and insignificant influence of terrigenous sources, resulting in the formation of rocks with oil-generating properties. During the regression periods, the terrigenous sedimentation increased along with the dissolved oxygen concentration, and deposits with low organic matter content and gas-generating properties were formed.

Idrisova et al. [3] elaborate the results of the above-mentioned study by focusing on the mineralogical, chemical, and isotopic characterization of pyrites from the rocks of the Bazhenov Formation (Upper Jurassic–Lower Cretaceous organic-rich shales, Western Siberia, Russia). Scanning electron microscopy reveals pyrites of different morphologies: small and large framboids, small crystals, and large euhedral crystals. Isotope ratio mass spectrometry and secondary ion mass spectrometry show isotopically light ( $\delta^{34}$ SCDT varying from –55 to –20‰) small framboids and microcrystalline pyrite, and isotopically heavy ( $\delta^{34}$ SCDT up to +26‰) large framboids and euhedral crystals of pyrite. The authors suggest the pyrite morphology and its sulfur isotope composition are controlled by the redox conditions and sedimentation regime. The accumulation of sediments that occurred under anoxic conditions links to the abundance of small framboids of pyrite, while the accumulation at suboxic conditions, possibly in the presence of oxygen, links to the presence of the large framboids and euhedral crystals of pyrite.

Yurchenko et al. [4] address the potential application of stable carbon and oxygen isotope composition of carbonates for the study of the organic-rich source rocks genesis on the example of the Upper Jurassic–Lower Cretaceous Bazhenov Formation (West Siberian Basin, Russia). The studied deposits are located in the central (the most productive) and peripheral (northern and southern) regions of the Bazhenov Formation distribution area, as an example of the different sedimentation conditions. The authors identify key factors influencing a stable isotope composition of carbonate minerals and establish its relation to the formation conditions. Using a thermodynamic model of carbon and oxygen isotope exchange in the carbonate–water–carbon dioxide system, the authors show that both isotopic composition of primary carbonates in sediments and the isotope exchange reactions with water and carbon dioxide (generated during the source rocks transformation) affect the isotope data for carbonates in the Bazhenov Formation together with other geochemical methods can be efficiently applied to determine sedimentation conditions and secondary alteration processes of oil source rocks.

Pedentchouk et al. [5] investigate the magnitude and direction of stable carbon and hydrogen isotope shifts of n-C<sub>15-30</sub> alkanes from a series of biodegraded oils sourced from kerogen Type II and mixed kerogen Type II/III. Compound-specific isotope data show a moderate <sup>13</sup>C-enrichment and no D-enrichment of n-alkanes in the most biodegraded oils from both types of source rocks. The authors conclude that the relatively homogeneous and sustained nature of C isotope composition of n-alkanes maintained during in-reservoir biodegradation indicates that these compounds have a good potential as a supplementary tool for oil–oil and oil–source rock correlation even in biodegraded oils. However, the labor-intensive cost-prohibitive H isotope methodology, as well as a high probability of D/H exchange during individual hydrocarbon generation and potentially subsequent equilibration with petroleum system waters, make the application of  $\delta D$  analysis far less attractive.

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Maturity calculations are very sensitive to temperature, as indicated by the double exponential dependence of maturity on temperature based on the Arrhenius equation. However, reconstruction of formation temperatures in the past requires reliable geothermal data on rock thermal properties and heat flow density. Popov et al. [6] demonstrate the first experience of supporting basin modeling in unconventional plays with advanced experimental geothermal investigations on the example of the Domanik Formation (Orenburg region, Russia). The rock thermal properties are both measured with continuous thermal core profiling on all recovered cores (~1.700), and determined from well-logging data within non-cored intervals. The influence of multiscale heterogeneity and anisotropy, in situ pressure and temperature, and core aging on the thermal properties of rock is accounted for. The authors show that the average value of the heat flow significantly (by more than 100%) exceeds the previously published value for this area, which corroborates reliable results from super-deep and deep scientific wells. The essential shortcomings of the methods and results of many previous geothermal investigations around the world lead to a necessity to reappraise these data to increase the quality of basin and petroleum system models.

Much attention is paid to the study of the kerogen chemical structure [7], variation of kerogen type on the depth [8], the interaction of the organic matter and mineral matrix [9], void space [10], and the kerogen-related multiscale heterogeneity and anisotropy [11] of the Bazhenov formation sediments.

Tanykova et al. [7] present results of kerogen chemical structure analysis directly in the Bazhenov Formation source rocks (West Siberia, Russia). The authors have developed new experimental procedures for semi-quantitative assessment of the organic matter content, composition, and distribution in the source rocks based on Fourier transform infrared (FTIR) spectroscopy in transmission and ATR modes, as well as FTIR microscopy of the rock surface. The application of the procedures has been verified using the data obtained by Rock-Eval pyrolysis and differential thermal analysis of the organic matter. The removal of carbonate minerals before the experiment expands the capabilities of the IR spectroscopy method for studying the structure of organic matter directly in rock without the preliminary stage of kerogen separation. FTIR microscopy (ATR, normalization method) used for organic matter surface distribution analysis reveals the heterogeneity of organic matter and mineral composition. The obtained results demonstrate the prospects of FTIR spectroscopy and microscopy for non-destructive and express analysis of the chemical structure and distribution of organic matter in rocks, including a study kerogen composition in organic-rich shales.

Bulatov et al. [8] have discovered the luminescent layers containing a significant amount of alginite in the Upper Jurassic–Lower Cretaceous Bazhenov Formation (West Siberia, Russia). The composition of the organic matter in so-called "alginite-rich layers" differs significantly from that in the organic-rich siliceous Bazhenov rocks. Rock-Eval pyrolysis, elemental analysis, bulk kinetics of thermal decomposition, and molecular composition of pyrolysis products indicate type I kerogen to be the predominant component of the organic matter. Analysis of the isotope composition of carbon, nitrogen, and sulfur provides insights into their origin and formation pathways. The layers proved to be good regional stratigraphic markers due to wide distribution over the central part of Western Siberia. The luminescence of the layers changes the color and intensity during maturation; this observation can be applied for maturity evaluation of the deposits from the immature stage to the middle of the oil window.

Bogdanovich et al. [9] discuss the issues of interaction of the organic matter and the siliceous–carbonate mineral matrix in organic-rich low-permeability rocks of the Upper Devonian Domanik Formation (Upper Kama Depression, Volga-Ural Basin, Russia). The authors identify intervals where organic matter can form a complex association with the siliceous–carbonate matrix using results of a complex study with light microscopy, X-ray diffraction analysis, scanning electronic microscopy, evaporation method, and the Rock-Eval pyrolysis. In some cases, the mineral carbonate matrix and the organic matter

form a one-whole high-molecular compound. It seems the organic matter is immobilized into the structure of the mineral carbonate matrix in the course of sedimentation. At the deposition and diagenesis stage, the carbonate matter interacts with acids of the organic matter and forms natural organo-mineral polymers. Water saturation, porosity, and geochemical properties of such polymers shed new light onto the problems of producing hard-to-develop nonconventional carbonate reservoirs and evaluating the associated risks.

Postnikova et al. [10] identify the types of void space in the sediments as well as the distribution patterns across the section of the researched wells drilled in five different areas of the Bazhenov formation (West Siberia, Russia). The deposits are represented by a wide complex of lithotypes, including various kinds of silicites, carbonate, clay rocks, and mixtites (the mineral composition of the rocks from different lithotypes was determined by X-ray diffraction analysis). The void space, studied by electron and optical microscopy, is a complex and hierarchically subordinated system, which includes voids and fractures of various sizes, configurations, and genesis. The authors show that elongated voids are confined to the upper part of the section, and isometric voids up to five microns in size are developed in the middle and lower parts of the section. The interlayers with high permeability, confined to the elongated pelecypod interlayers, are identified. An orthogonal system of fractures connecting voids of various sizes, shapes, and genesis into a single hydrodynamic system is substantiated. The void space is characterized by a fairly high degree of spatial heterogeneity, which is controlled by lithological, facies, and tectonic factors, as well as the direction of catagenetic processes.

Chekhonin et al. [11] focus on the study of high multiscale heterogeneity and anisotrop y, natural in unconventional formations, which complicate reservoir characterization and dictate the sampling methodology used. Rocks from the Bazhenov Formation (West Siberia, Russia) are studied via the integration of continuous high-resolution thermal measurements with an optical scanner and scratcher along the core column. The authors describe features of the suggested integration and quantify the formation heterogeneity at different scales (from mm to meters) for two physical properties: unconfined compressive strength (UCS) and thermal conductivity. Observed positive correlations between these properties, unique to the different rock types, make it possible to partially replace the semidestructive scratch test with non-destructive optical scanning, providing UCS estimation. Thermal conductivity, as opposed to UCS, is more sensitive to a change in the content of organic matter than to a change in the content of clays. It sheds light on a way to distinguish the independent effects of clay and kerogen. As the integration of thermal core profiling and scratch testing data looks promising for unconventional reservoir characterization, the authors give recommendations regarding how to organize future works.

Currently, the development of unconventional resources has not been performed without using advanced methods including hydraulic fracturing and/or thermal EOR methods. This forces specialists to carry out additional special studies on the core, providing necessary information for modeling, which is the subject of the last two articles of the Special Issue.

Bobrova et al. [12] present a new methodology for rock sample hydraulic fracturing under pseudo-triaxial loading conditions representing stressed reservoir conditions. After preliminary testing on sandstone, the methodology is applied to study the dynamics of hydraulic fracture propagation in six shale-like core samples from the subsalt complex (Volgograd region, Russia). A linear correlation of the breakdown pressure with the tensile strength of the sample and the speed of fracture growth is observed. Deviations from the general relationships observed for three samples are explained by the influence of the rock matrix features. The authors separate acoustic emission signals with a dominant shear component from the signals with a significant tensile component using the analysis of the moment tensor inversion of radiated signals. Determined planes of the main fractures agree with the results of the post-test X-ray CT analysis. The combination of several independent laboratory techniques allows specialists to determine the parameters that can be used for the verification of hydraulic fracturing models. Chekhonin et al. [13] describe a full set of advanced methods and equipment for obtaining reliable data on thermal properties at atmospheric and reservoir conditions, as well as a new, vast set of experimental data obtained from the Karabikulovskoye heavy oil field (Russia). The results of comparing obtained data with those published, as well as the findings from long-term authors' study in thermal petrophysics, clearly indicate the traditional underestimation of the existing uncertainty in data on the thermal properties used for modeling. Moreover, the authors show that software capabilities for the integration of these data are limited, outdated in some aspects, and require revision. Observed significant (by tens of percent) errors in the evaluation of the cumulative oil production and steam/oil ratio caused by the lack of experimental data are a clear signal to the community. This means that both experimental study of thermal properties with modern technologies and improving simulators for a proper account of experimental data are necessary steps to increase the quality of thermal EOR modeling.

The great majority of articles in this Special Issue are devoted to petrophysics and geochemistry of unconventional reservoirs in Russia related to the Domanik Formation in the Volga–Ural Basin and the Bazhenov Formation in the West Siberian Basin, which is the largest petroleum basin in the world. Nevertheless, we believe that the key findings, as well as new ideas, concepts, and methods, can be useful for specialists over the world and are of broad international interest.

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