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Modeling of Thermodynamic Processes for Assessing Hydrocarbon Systems at Depths Exceeding 5 km

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ABSTRACT

The discovery of oil reservoirs at great and ultra-great depths has necessitated a revision of existing concepts about the possibility of hydrocarbon generation and preservation under extremely high pressure–temperature conditions. This work analyzes geochemical approaches and basin modeling methods used for predicting hydrocarbon generation at great depths. It examines the influence of high temperatures and pressures, burial rate, phase transitions, and other factors on the formation and destruction of oil and gas. An analysis of deep hydrocarbon systems is performed, and the potential of thermodynamic modeling of fluid equilibrium compositions and the results of experiments on oil transformation under high P–T conditions are considered. A modern approach to assessing a high-organic-carbon (Domanik) formation is presented, which allows evaluation of hydrocarbon generation potential. The reasons why existing geochemical methods and basin modeling can yield inconclusive results for similar processes at great depths under extreme pressure–temperature conditions are identified. In particular, sources of uncertainty in hydrocarbon phase transitions are discussed, associated with a lack of experimental data for model calibration and the limitations of thermodynamic models beyond their validated ranges, among other factors.

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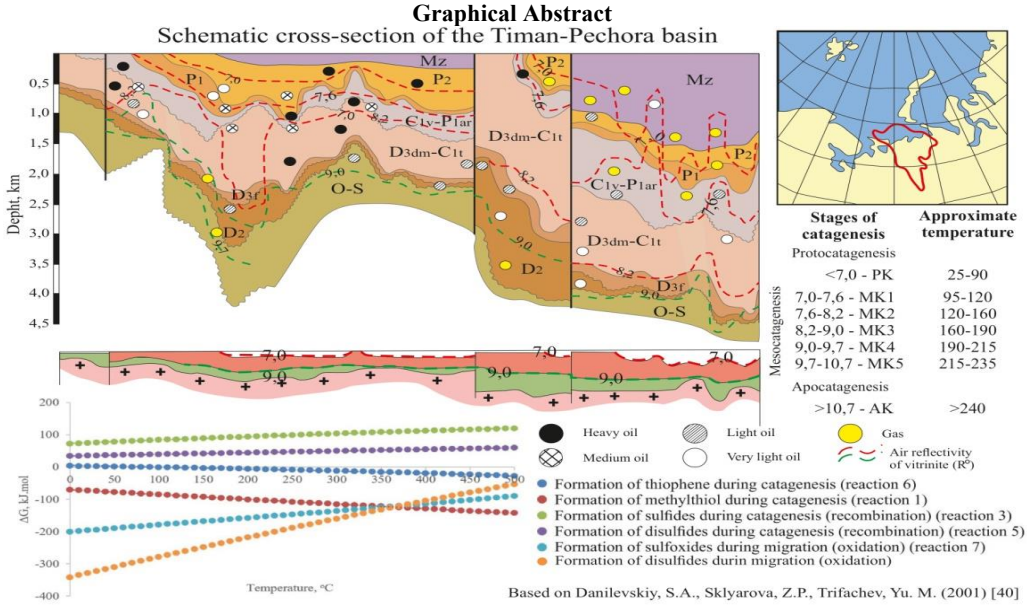
Graphical Abstract



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NOMENCLATURE

HC	hydrocarbons	R_2NH	Amines
R-SH	Thiols	R_3N	
R-S-R'	Sulfides	R-COOH	Carboxylic acids
R-S-S-R'	Disulfides	Ar-OH	Phenols
R-SO-R'	Sulfoxides and sulfones	R-OH	Alcohols
$R-SO_2-R'$		R-COO-R'	Esters
$R-NH_2$	Amines	R-CO-R'	Ketones

1. INTRODUCTION

Recently discovered oil and gas reservoirs at great and ultra-great depths (1), as well as indirect evidence of reservoirs existing in supercritical fluid conditions, force a reconsideration of theoretical ideas about the conditions for the formation and preservation of hydrocarbons (HC) in zones of high pressure and temperature (2-4). The most discussed issues in this context include: the influence of thermobaric (pressure–temperature) conditions on hydrocarbon formation and destruction; the influence of the rate and magnitude of rock subsidence and uplift on HC generation and redistribution; determining criteria and threshold values for phase transitions in hydrocarbon systems; the influence of the initial organic matter composition and maturity (kerogen type) on the phase composition of generated hydrocarbons; the influence of kinetic parameters of bitumoids on phase ratios and phase transition conditions; the influence of the lithological composition and depositional environment of kerogen-bearing strata on their hydrocarbon potential, and on migration and accumulation conditions; the influence of overlying salt-bearing strata and deep conductive faults (which significantly alter the distribution of geothermal and hydrostatic gradients) on the character and maximum depth of oil and gas asccumulations (5-7); the contribution of "deep" methane to the formation of HC accumulations, including high-molecular-weight compounds (8-10). Only a comprehensive examination of these issues will yield new practical results and technologies for discovering hydrocarbon deposits at great and ultra-great depths.

However, the practical applicability of theoretical models at such conditions remains unproven. The question arises whether it is possible to create a technology aimed at exploring oil and gas reservoirs at ultra-great depths and how effective it could be in the foreseeable future. Other possible approaches include experimental testing of various models of HC formation and accumulation under extreme conditions (with validation against core and fluid data), as well as the search for geochemical halos of dispersion from deep HC accumulations (11, 12).

Debates about the origin and migration of oil have catalyzed extensive experimental research, new ideas and knowledge, identification of factors affecting oil and gas quality, and the development of new investigative methods that were later implemented in oil and gas exploration technologies. The foundation of these technologies was new theoretically grounded material balance equations that do not contradict the laws of physics and chemistry, enabling calculation of volumetric ratios between initial organic matter and generated hydrocarbons (13-15). Subsequently, numerical modeling tools for sedimentary basin evolution were created on this basis, which are effectively used to predict and assess potential oil and gas presence.

The depletion of large conventional oil and gas traps in recent decades has led to a decline in exploration efficiency, which in turn spurred a comprehensive analysis of all processes of oil and gas formation. Such analysis includes determining the conditions for organic matter accumulation in sedimentary basins, the influence of temperature and pressure during burial of organic-rich deposits, the pathways of hydrocarbon fluid migration, and the delineation of zones of HC accumulation vs. dissipation. The development and implementation of basin modeling technologies in exploration practice have significantly improved the success rate of assessing petroleum potential (16-18).

The emergence of a new resource base in the form of low-permeability shale and carbonate reservoirs in the early 21st century forced a revision of ideas about migration as a stage of petroleum formation. At the same time, interest increased in technologies for enhancing rock porosity and permeability (hydraulic fracturing). Meanwhile, the theory of oil formation continued to evolve thanks to detailed studies of oil-bearing strata containing mobile but not yet expelled hydrocarbons (19-21).

Analysis of the influence of the above factors on the evaluation of petroleum potential in deep-seated complexes, taking into account new research and achievements (primarily in Chinese sedimentary basins such as the Tarim, Junggar, Ordos, Sichuan basins; as well as the Gulf of Mexico and Brazil's Santos Basin), has made it possible to identify potential areas for studying hydrocarbons at great and ultra-great depths in sedimentary basins and large depressions of Russia (22-24). Thermobaric and historical-geological criteria for the prospects of deep complexes were formulated, and a methodology for their detailed study was proposed (2). This methodology includes geochemical analyses of

hydrocarbons and their sources (pyrolysis, chromatography), lithological and petrophysical core studies – all aimed at assessing the probability of oil and gas presence in deep horizons and subsequently pinpointing the most promising drilling targets.

The problem of the genesis of hydrocarbons and the conditions for formation and preservation of deposits has not only theoretical but also important practical significance. Proposed approaches to this problem often reflect researchers' personal views on the origin of oil and natural gas, based on two fundamentally different hypotheses: the sedimentary-migrational hypothesis versus the deep mineral-mantle genesis hypothesis.

At present, among modern petroleum generation hypotheses developed within the biogenic-sedimentary paradigm, opinions are increasingly emerging that emphasize the significant role of energy and material from the Earth's deep zones. Examples include the geofluidodynamic concept (25), the geosynergetic concept of natural hydrocarbon-generating systems (26), the sedimentary-inorganic hypothesis (27), and others. According to these works, fluxes of deep fluids stimulate the process of petroleum generation, the expulsion of hydrocarbons from the organic matter of sedimentary strata, and promote their accumulation.

Thus, in order to model the conditions of HC accumulation at great depths, one must take into account hydrocarbon genesis and consider reservoir formation from the following perspectives. First, there is the viewpoint that some indeterminate portion of hydrocarbons could have formed in a high-temperature (>200–250 °C) zone of organic matter transformation due to the combination of high temperature–pressure and a specific organic matter composition. Second, some contribution is associated with inorganic synthesis of hydrocarbons in zones where hydrogen and carbon are transported from the deep interior under certain thermobaric conditions (perhaps it is more accurate here to speak of an energetic contribution to process intensity).

To date, the problem of hydrocarbon compound formation via a combination of organic and inorganic processes remains unresolved. One cannot dismiss the thesis that the indicators of oil "biogenicity" may be explained by the fact that during migration from deep horizons, primary hydrocarbons "wash" the organic matter of sedimentary rocks, acquiring some properties and components of both the sedimentary strata and the organic matter.

In most petroleum basins, the shallow (upper) complexes are generally already explored, and searching for oil/gas in the deeper parts of the sedimentary cover has become a new, independent direction of study (28, 29). It is hard to agree with the opinion that every structure containing oil and gas in the shallow sedimentary sequence is also suitable for finding oil and gas in the deep horizons, including in the crystalline basement.

In recent years, with advances in computing, the capabilities of basin modeling have expanded, improving prediction accuracy and reducing uncertainty in exploration. Modern software suites can account for more and more factors and processes, approaching a realistic picture of the formation of deep petroleum systems.

It must be emphasized, however, that even the most advanced models today encounter difficulties when applied to the extreme conditions of ultra-deep petroleum generation zones.

1. 1. Limitations of Methods under Extreme Pressure–temperature Conditions Despite significant progress in understanding petroleum generation, current geochemical methods and basin modeling have limited applicability at great depths (>5–6 km) under extremely high temperatures and pressures. Below are the main problems that arise when attempting to predict the state of hydrocarbon systems under such conditions:

• Uncertainty of hydrocarbon phase transitions. Under standard sedimentary basin conditions, the range of HC phase states is relatively well studied: it is known at what temperatures and pressures oil transitions to condensate and gas, and when solid residues (pyrobitumens) form. However, at great depths (temperature on the order of 250–300 °C and pressure of hundreds of MPa), phase equilibria shift substantially. In this realm, the existence of supercritical fluids is possible, where the distinction between liquid and gas virtually disappears. The absence of clear phase boundaries complicates prediction: for example, it is not obvious whether oil remains liquid or fully transitions into a gaseous supercritical phase under such parameters. The critical parameters of hydrocarbons can change greatly with increasing molecular weight and presence of impurities. Consequently, standard oil and gas phase diagrams extrapolated to ultra-high pressures carry large uncertainty. In practice, this means we cannot say with confidence whether at a depth of 7–8 km liquid oil will be present, or if the hydrocarbon mixture exists as a single gas-like (supercritical) phase, or if it separates into gas and a solid carbon residue. Such phase transitions remain largely hypothetical due to a lack of empirical data.

• Lack of experimental data. Experimentally reproducing conditions of ~200–300 °C and >100 MPa in the laboratory is very difficult, especially to maintain for extended periods even remotely comparable to geologic time. The few experiments conducted with oil and organic matter at high P–T have yielded valuable information, but these data are clearly insufficient to fully calibrate models. Many key parameters – e.g. kerogen decomposition rates at 250–300 °C, hydrocarbon

solubility in water at 100–200 MPa, diffusion properties of supercritical fluids, etc. – remain poorly studied. The absence of an experimental basis forces models to extrapolate patterns established at lower temperatures (say, 100–150 °C) to the high-temperature realm, which may be invalid. As a result, predictions may differ depending on the chosen kinetic scheme or thermodynamic model, and confidence in them is low. We must recognize that our understanding of real petroleum system behavior at ultra-high pressures is still largely theoretical rather than based on direct experiment.

• Mismatch of thermodynamic models with real systems. Equilibrium composition models rely on a simplified representation of oil, gas, and kerogen as a few quasi-pure substances with given properties. This simplifies calculations, but real oil consists of hundreds of components, and under extreme conditions new reactions may occur that the model doesn't include. For example, further compaction of hydrocarbons into solid carbon phases (graphite formation) or interactions with the mineral matrix (e.g. hydrogen being sequestered into minerals or fluids) may occur. Existing equations of state for petroleum fluids, calibrated up to ~150 °C and a few tens of MPa, can produce large errors at 300 °C and 100+ MPa. Thermodynamic parameters of many heavy components at such conditions are simply unknown. Moreover, in the supercritical region the very notions of "oil" and "gas" lose clarity – instead of a two-phase system, there may be a single supercritical phase, and standard two-phase models cease to work. Thus, thermodynamic models require serious expansion and verification for application to ultra-deep levels.

• Limitations of kinetic models in basin modeling. Kinetic models of hydrocarbon generation (for example, the model by Pepper and Corvi (30)) are based on experimental kerogen pyrolysis at temperatures up to ~500 °C, from which decomposition parameters are extrapolated to geological timescales. These models work well up to the end of the "oil window" (~150–180 °C, catagenesis up to stage MK5). But at significantly higher temperatures (200–250 °C and above) the reliability of such models decreases. It is possible that at 250–300 °C, with prolonged heating, alternative pathways of organic decomposition occur, yielding products (e.g. methane and carbon) in proportions different from those predicted by standard kinetics. Moreover, kinetic parameters obtained from short-term heating of samples may be inadequate for describing reactions under slow heating over millions of years. Consequently, basin models may under- or over-estimate gas generation at great depths. For example, "secondary gas generation" from already formed oil during prolonged heating may occur, which is not always accounted for in modeling software.

• Other factors and uncertainties. It should be noted that at great depths abnormally high pore pressures are often present, affecting fluid migration and trap preservation – models need to incorporate mechanical processes and rock instability. The role of natural catalysts (e.g. minerals whose surfaces can facilitate HC decomposition reactions) at high temperatures is not fully clear – some minerals might accelerate or retard oil cracking, shifting stability limits. Furthermore, under extreme conditions the role of hydrogen and hydrogen-bearing fluids emanating from the deep mantle may increase. An influx of hydrogen could lead to hydrogenation of carbon residues, theoretically generating heavy hydrocarbons even at high temperatures – though this is a hypothetical mechanism requiring verification. Finally, the pore structure at depth is greatly altered: pores and fractures are partly closed due to high pressure and diagenesis, affecting hydrocarbon mobility and potentially hindering migration or, conversely, creating conditions for local preservation in isolated traps.

Thus, existing methods of forecasting petroleum systems must be used with great caution when extending to depths beyond 5–6 km. Further development of theoretical models is necessary, along with the accumulation of experimental data under conditions close to real high P–T, and possibly a revision of some fundamental assumptions about the limiting conditions of oil formation. Only a combination of different approaches – thermodynamic, kinetic, and geophysical – and their cross-calibration will gradually reduce uncertainty and improve the reliability of predictions of oil and gas presence at the greatest depths.

Generalizing the experience of determining the conditions of HC accumulations at great depths, together with modeling the possibility of HC formation and preservation under ultra-harsh thermobaric conditions at great and ultra-great depths, will lead to the creation of a technology no less effective than basin modeling, which enabled the discovery and assessment of enormous oil and gas reserves at shallow and moderate depths.

It should be noted that the modern basin modeling approach to petroleum generation is developing in parallel with an equilibrium approach based on kinetic models of kerogen decomposition, which allows one to account for the non-equilibrium nature of real geological processes.

In this paper, the results of applying geochemical methods to the problem of predicting petroleum systems at great depths are considered. The fundamentals of thermodynamic (equilibrium) modeling of the composition of hydrocarbon fluids and the results of a geochemical study of a specific region are presented. Current approaches to basin modeling of petroleum systems are outlined. The final section of the paper is devoted to a discussion of the use of existing methods under the extremely high temperatures and pressures characteristic of ultra-deep zones.

2. MATERIALS AND METHODS

2. 1. Thermodynamic Modeling as the Basis for Predicting Ultra-deep Hydrocarbon Deposits

Numerous studies of formation fluids show that up to temperatures of about 320 °C, the composition and aggregate state of oil remain relatively stable. However, with further temperature increase – in the range of 350–380 °C – especially at pressures close to the saturated vapor pressure of the oil's components (~150 MPa), active thermolysis begins with the formation of methane, propane, butane, and carbon dioxide. At the same time, the proportion of light fractions increases, transitioning into the gas phase as condensate, known as "invisible oil." Under these conditions, solid bitumen also forms. By 550–600 °C, virtually all organic matter decomposes to methane and a solid carbon residue — anthraxolite. These observations highlight the significant influence of the combined effect of temperature and pressure on the onset of thermal cracking: under abnormally high reservoir pressure, this process shifts to higher temperatures, allowing oil to remain liquid even under conditions traditionally considered unfavorable for its existence.

Thermodynamic modeling based on empirical data from core analyses is widely used to analyze phase states and determine the pressure–temperature conditions of formation and evolution of hydrocarbon accumulations at significant and ultra-deep horizons. The primary assumption of this approach is the possibility of local equilibrium in geochemical systems, which justifies the use of equilibrium thermodynamics to calculate the composition of natural fluids. As numerous studies show, this assumption is valid at very high temperatures (above 150–200 °C) or over long process durations. Key assumptions used in kinetic modeling are given in Table 1.

The theoretical foundation of the method was laid by Gibbs (31). Modern approaches to calculating the equilibrium composition of real systems are divided into direct and combined methods. Direct methods focus on determining equilibrium parameters directly, whereas combined methods are used to model equilibrium compositions in non-ideal systems. Since in geological settings pressure and temperature often remain constant, isobaric-isothermal conditions are applicable in most phase behavior models. The modeling utilized an in-house code based on Gibbs energy minimization under specified P–T conditions. Thermodynamic constants were sourced from the SUPCRT92 database (32) and updated parameters from Helgeson et al. (14).

One of the main tools for quantitative analysis of such processes has been the method of thermodynamic potentials (30, 33, 34), which was actively used in earlier geochemical works (31). This method made it possible to delineate stability regions of various products of organic matter transformation — the so-called geochemical facies. The approach is based on the concept from Helgeson et al. (14) that the transformation of biomass occurs sequentially: first into bitumen, then kerogen, and thereafter into liquid hydrocarbons and gas. Thus, oil and gas formation can occur at higher pressures,

TABLE 1. Key assumptions used in kinetic modeling

Assumption	Limitations	Implications for Modeling	Potential Mitigation Approaches
Uncertainty of phase transitions	Lack of clear boundaries between liquid, gas, and supercritical phase at T > 250 °C, P > 100 MPa	Inability to unambiguously determine the phase state of a hydrocarbon mixture (oil/gas/supercritical fluid)	Use of experimental PVT data at high P–T conditions; application of equations of state suitable for supercritical conditions
Lack of experimental data	Limited number of laboratory studies under prolonged exposure to conditions T >250 °C and P >100 MPa	Extrapolation of kinetic and thermodynamic parameters beyond validated ranges	Conducting new experiments on kerogen and oil thermolysis in autoclaves with long exposure times
Limitations of thermodynamic models	Use of a simplified hydrocarbon phase composition instead of real multicomponent mixtures	Underestimation or overestimation of the stability of heavy fractions, heteroatomic compounds, and solid residue	Integration of more detailed compositional models
Challenges in kinetic modeling	Kinetic parameters derived from short-term heating experiments, not accounting for geological time scales	Inaccurate prediction of gas generation rates and oil cracking at great depths	Development of kinetic schemes based on geologically relevant experiments
Influence of mineral matrix and catalysts	Failure to account for the catalytic action of clay minerals or oxides at high T–P	Incorrect assessment of thermolysis pathways and product composition	Inclusion of mineral-mediated reactions in the model; laboratory tests for catalytic activity at high P–T
Role of deep-seated fluids (H_2, CO_2, etc.)	Lack of accounting for the influx of hydrogen or carbon from mantle or metamorphic sources	Omission of possible oil stabilization mechanisms or hydrocarbon synthesis in deep zones	Integration of geodynamic models accounting for tectonic faults and vertical fluid flows

temperatures, and depths exceeding the classical limits of petroleum generation. The model relies on fundamental laws of thermochemistry — Hess's law, Kirchhoff's law, and the second law of thermodynamics. Solving the system of chemical equilibrium equations at various P–T parameters allows one to construct depth profiles of component distribution and predict the stability zones of oil and gas accumulations in sedimentary basin cross-sections, including in deeply buried levels.

The results obtained are based on data from the Domanik deposits of the eastern Siberian Platform and the Tarim and Sichuan basins, these data include Rock-Eval pyrolysis, chromatography, fluid composition, and petrophysical properties (2, 3, 22).

3. THERMODYNAMIC MODELING FOR PREDICTING HYDROCARBON SYSTEMS AT GREAT DEPTHS

3. 1. Mechanisms and Thermodynamic Feasibility of Generation of Hydrocarbons and Heteroatomic Components from Kerogen The chemical composition of a formation fluid generated during catagenesis at various depths, and the degree of transformation of its components, will depend on the type of initial kerogen, the pressure–temperature conditions of its breakdown, the rate at which the kerogen is buried, the introduction into the fluid of various substances formed during deep geological processes (for example, hydrogen), the conditions of migration of matter to the surface, and the reservoir conditions (Figure 1).

During catagenesis, kerogen components form the composition of the future crude oil, including hydrocarbons: alkanes, naphthenes, and arenes. These compounds arise from the thermal cleavage of complex organic kerogen molecules such as lipids, proteins, or carbohydrates. Chemically, the catagenesis process involves radical cleavage reactions, recombination, cyclization, and aromatization.

Nitrogen-containing oil components are generated by the breakdown of nitrogenous functional groups present in the kerogen structure (36). Nitrogen in kerogen exists in the form of amines, amides, pyrroles, pyridines, porphyrins, and other heterocyclic structures, which upon thermolysis convert into various nitrogen-containing oil compounds. The main classes of such compounds include amines, pyridines, pyrroles, quinolines, carbazoles, porphyrins, and their derivatives, as confirmed by high-resolution mass spectrometry data (36).

Sulfur-containing oil components are produced by the breakdown of sulfur-containing functional groups. Sulfur in kerogen is present in functional groups that, upon thermolysis and subsequent reactions, yield sulfur-containing oil compounds. These include thiols (mercaptans), sulfides, disulfides, thiophenes, and their derivatives.

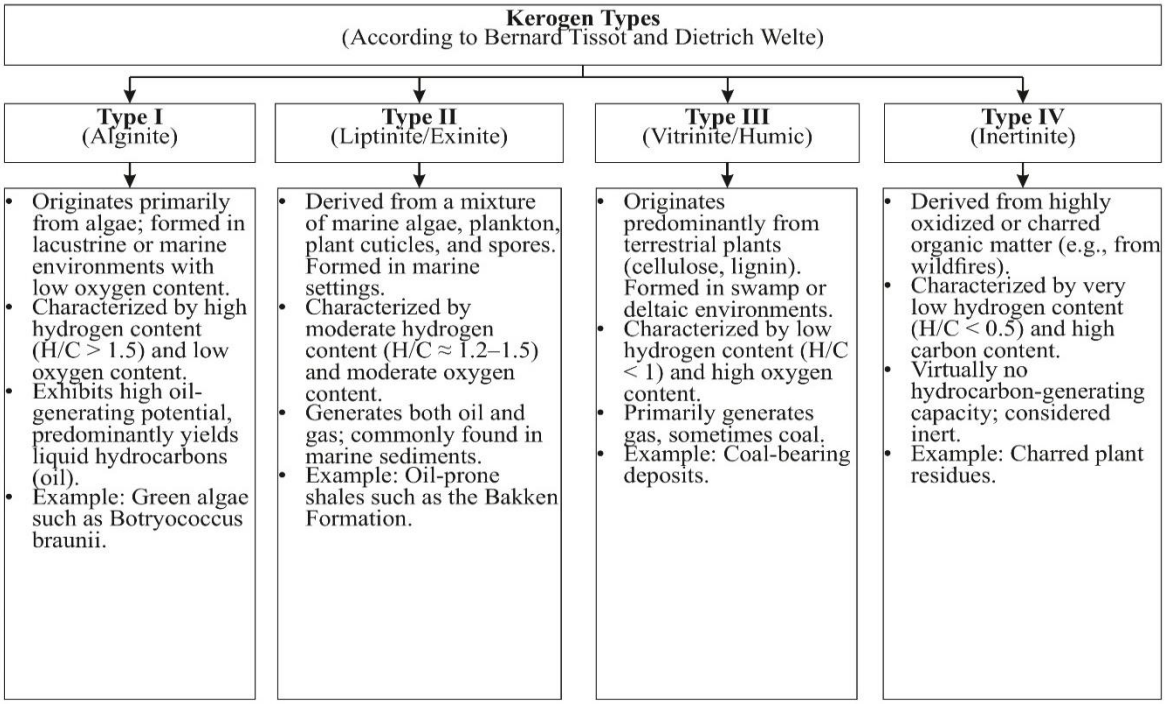

Figure 1. Classification of kerogen types according to Bernard Tissot and Dietrich Welte (35)

Oxygen-containing oil components also form during catagenesis through the breakdown of oxygen-containing functional groups in the kerogen structure. Kerogen contains oxygen in the form of carboxyl, hydroxyl, ether, carbonyl, and other groups, which upon thermolysis transform into various oxygen-containing oil compounds. The main classes of such compounds include carboxylic acids, phenols, alcohols, ethers, ketones, aldehydes, and furans.

Typical classes of heteroatom compounds are shown in Figure 2.

During the formation of liquid hydrocarbons from the parent kerogen, the following key reactions can be identified. Thermolysis of kerogen is accompanied by the cleavage of C–C, C–O, C–N, and C–S bonds, resulting in the formation of free radicals or unsaturated molecules.

The presence of sulfur-containing components in crude oil can serve as an indicator of the degree of kerogen transformation. As hydrocarbons are progressively formed, sulfur compounds derived from oil-prone kerogen can be detected, and their formation can be described by the following principal reactions:

Thermolysis of kerogen, involving the cleavage of C–S, S–S, and S–H bonds and the generation of reactive radicals or molecules containing sulfur atoms.

Radical reactions, including recombination of the formed radicals and their interaction with hydrocarbons or hydrogen, leading to the formation of new sulfur-containing compounds.

High-temperature cyclization and aromatization of sulfur-bearing molecules, resulting in the formation of heterocyclic compounds such as thiophenes.

Secondary reactions of recombination, oxidation, or reduction, leading to the generation of more complex sulfur-containing structures.

Thiols are formed via cleavage of weak S–S or C–S bonds in kerogen followed by hydrogen addition (Reaction 1):

$$\begin{aligned} &\text{R-S-S-R'} + H_2 \rightarrow \text{R-S-H} + \text{H-S-R'} \\ &C_2H_6S_2 + H_2 \rightarrow 2CH_4S \end{aligned} \quad (1)$$

Sulfides are formed by oxidation of thiols and interaction with hydrocarbons (Reaction 2) or by radical recombination (Reaction 3):

$$\begin{aligned} &\text{R}\bullet + \bullet\text{S-R'} \xrightarrow{[O]} \text{R-S-R'} + H_2O \\ &CH_4 + CH_3\text{-HS} + O_2 \xrightarrow{[O]} CH_3\text{-S-}CH_3 + H_2O \end{aligned} \quad (2)$$

$$\begin{aligned} &\text{R}\bullet + \bullet\text{S-R'} \rightarrow \text{R-S-R'} \\ &C_2H_6 + CH_3HS \rightarrow C_2H_5\text{-S-}CH_3 + H_2 \end{aligned} \quad (3)$$

Disulfides form via oxidation of thiols (Reaction 4) or recombination of thiyl radicals (Reaction 5):

$$\begin{aligned} &\text{R-S}\bullet + \bullet\text{S-R'} \xrightarrow{[O]} \text{R-S-S-R'} + H_2O \\ &CH_3\text{-HS} + CH_3\text{-HS} \xrightarrow{[O]} CH_3\text{-S-S-}CH_3 + H_2O \end{aligned} \quad (4)$$

$$\begin{aligned} &\text{R-S}\bullet + \bullet\text{S-R'} \rightarrow \text{R-S-S-R'} \\ &C_2H_5\text{-HS} + CH_3\text{-HS} \rightarrow C_2H_5\text{-S-S-}CH_3 + H_2 \end{aligned} \quad (5)$$

Thiophenes and their derivatives are generated through cyclization of sulfur-containing molecules followed by aromatization (37). The formation of thiophene (Reaction 6) is characteristic of more advanced stages of catagenesis.

$$CH_2{=}CH\text{-}CH{=}CH_2 + H_2S \rightarrow C_4H_4S + 2H_2 \quad (6)$$

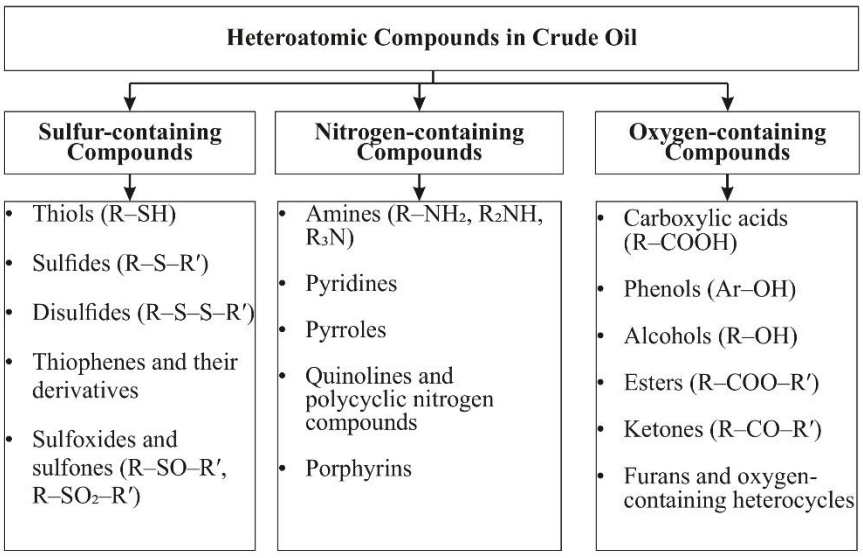

Figure 2. Classification of typical heteroatomic compounds included in formation fluids

More complex thiophenes, such as benzothiophene, arise from the condensation of aromatic hydrocarbons with sulfur-containing fragments.

Sulfoxides (Reaction 7) and sulfones (Reaction 8) form predominantly during the migration of the reservoir fluid to the surface via oxidation of sulfides in the presence of oxygen or other oxidants in pore waters.

$$\text{R-S-R'} \xrightarrow{[O]} \text{R-SO-R'}$$
$$\text{C}_2\text{H}_6\text{S} \xrightarrow{[O]} \text{C}_2\text{H}_6\text{OS} \quad (7)$$

$$\text{R-SO-R'} \xrightarrow{[O]} \text{R-SO}_2\text{-R'}$$
$$\text{C}_2\text{H}_6\text{OS} \xrightarrow{[O]} \text{C}_2\text{H}_6\text{O}_2\text{S} \quad (8)$$

For the above reactions, the Gibbs free energy changes as a function of temperature were calculated and are presented in Figure 3. The curves were calculated using standard thermodynamic data (ΔH°f, S°, Cp) from reference sources (15, 32) with extrapolation based on temperature-dependent heat capacity equations. The pressure was assumed to be 100–150 MPa, typical for depths of 5-7 km. The methodology used for these calculations is described by Cheremisina et al. (38).

From the obtained dependencies, it can be concluded that thiol formation is spontaneous throughout all stages of catagenesis. The formation of thiophene and its derivatives becomes feasible in high-temperature zones provided sufficient hydrogen sulfide is present. The formation of sulfides, disulfides, sulfoxides, and sulfones is only possible in the presence of oxidants and is most likely to occur during the migration of reservoir fluids toward the surface and their localization within reservoir traps.

Thus, the key factors governing the compositional profile of the reservoir fluid include the type of kerogen undergoing catagenesis and the pressure–temperature conditions under which catagenesis occurs. The effects of these parameters are summarized in Tables 2 and 3 (39).

3. 2. Interaction of Oil Components with Hydrogen Introduced into the Reservoir by Geological Processes

Earlier work, Prishchepa et al. (2) examined the mutual transformations of hydrocarbons in the presence of hydrogen under various reservoir conditions. In the present work, emphasis is placed on investigating similar transformations for a number of sulfur-containing compounds. Reactions of hydrodesulfurization of sulfur-containing compounds by hydrogen entering the reservoir have been observed in natural systems and confirmed by modeling (40, 41).

In these processes, thiols react with hydrogen to form the corresponding hydrocarbon and hydrogen sulfide. This reaction proceeds relatively easily due to the weak C–S bond (Reaction 9):

$$\text{R-SH} + \text{H}_2 \rightarrow \text{R-H} + \text{H}_2\text{S}$$
$$\text{CH}_3\text{-SH} + \text{H}_2 \rightarrow \text{CH}_3\text{-H} + \text{H}_2\text{S} \quad (9)$$

Sulfides are cleaved by hydrogen to form two hydrocarbon molecules and hydrogen sulfide. This reaction requires more severe conditions than for thiols (Reaction 10):

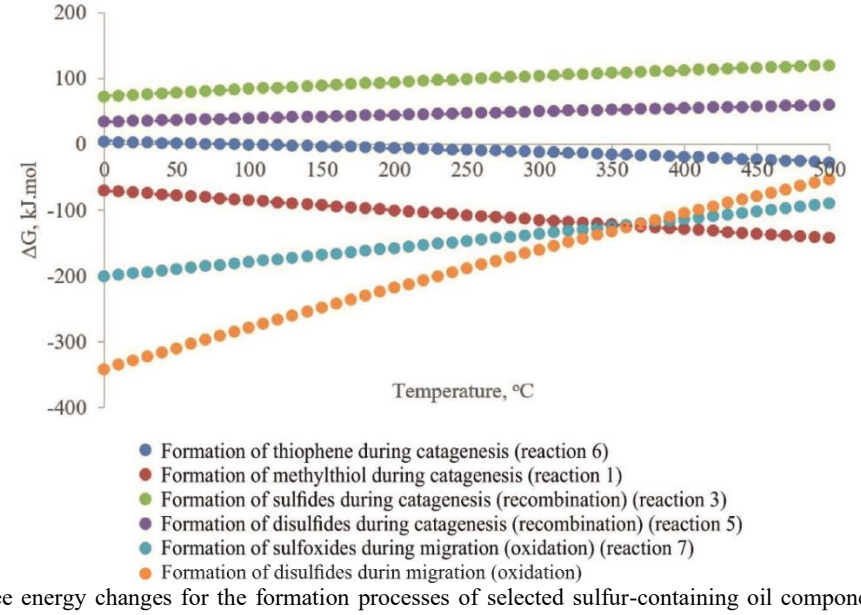

Figure 3. Gibbs free energy changes for the formation processes of selected sulfur-containing oil components as a function of temperature

TABLE 2. Effect of kerogen type on the formation of hydrocarbons and heteroatomic components of oil

Kerogen Type	Hydrocarbons	Sulfur-containing components	Oxygen-containing components	Nitrogen-containing components
Type I (algal)	Rich in lipids, generates a large amount of alkanes and naphthenes and a smaller quantity of arenes (aromatic hydrocarbons).	Low sulfur content; hydrocarbons predominate.	Low oxygen content; hydrocarbons predominate, but alcohols and carboxylic acids can form from lipids.	High nitrogen content (up to 2–3%) due to high protein and chlorophyll content, leading to the formation of porphyrins and amines.
Type II	Contains lipids and cyclic structures, forming a mixture of alkanes, naphthenes, and a moderate amount of arenes.	High sulfur content (up to 10–15%); generates a large amount of thiols, sulfides, and thiophenes.	Moderate oxygen content; carboxylic acids, esters, and furans are formed.	Moderate nitrogen content; pyrroles, pyridines, and quinolines predominate.
Type III	Rich in lignin, which promotes formation of arenes and yields fewer alkanes and naphthenes.	Low sulfur content and few sulfur-containing compounds.	High oxygen content (up to 20–30%) due to lignin and cellulose; phenols and furans predominate.	Low nitrogen content; nitrogen-containing compounds are minimal, mostly amines and simple heterocycles.

TABLE 3. Effect of temperature on the formation of hydrocarbons and heteroatomic components of oil

Kerogen transformation temperature (°C)	Hydrocarbons	Sulfur-containing components	Oxygen-containing components	Nitrogen-containing components
100-150	Predominant formation of alkanes and naphthenes via cracking and cyclization	Mainly thiols and sulfides form.	Primarily carboxylic acids, alcohols, and esters form.	Amines and simple heterocycles (pyrroles, pyridines) form
150-300	Increased proportion of arenes (aromatics) due to dehydrogenation and aromatization.	Growing proportion of thiophenes and derivatives due to aromatization.	Decarboxylation and dehydration reduce the content of oxygen-containing compounds, increasing the share of furans and phenols.	Formation of more complex structures (quinolines, carbazoles) through aromatization.

$$\begin{aligned} &R\text{-}S\text{-}R + H_2 \rightarrow 2R\text{-}H + H_2S \\ &CH_3\text{-}S\text{-}CH_3 + H_2 \rightarrow 2CH_4 + H_2S \end{aligned} \quad (10)$$

Disulfides, under hydrodesulfurization, split into two hydrocarbons and two molecules of hydrogen sulfide. The S–S bond is broken, and each sulfur is removed as H_2S (Reaction 11):

$$\begin{aligned} &R\text{-}S\text{-}S\text{-}R + 3H_2 \rightarrow 2R\text{-}H + 2H_2S \\ &CH_3\text{-}S\text{-}S\text{-}CH_3 + 3H_2 \rightarrow 2CH_4 + 2H_2S \end{aligned} \quad (11)$$

Thiophenes are compounds resistant to hydrodesulfurization because of the aromatic nature of the ring. The reaction requires higher temperatures and active catalysts. The thiophene ring is first hydrogenated, then cleaved, forming hydrocarbons and H_2S (Reaction 12):

$$CH_3\text{-}S\text{-}S\text{-}CH_3 + 3H_2 \rightarrow 2CH_4 + 2H_2 \quad (12)$$

Complex polycyclic sulfur-containing compounds (e.g., dibenzothiophene derivatives) are resistant to hydrodesulfurization due to their complex structure. These reactions require even more severe conditions, and often partial hydrogenation of rings occurs before sulfur removal. Products depend on the structure of the starting compound, but they are usually polyaromatic hydrocarbons and H_2S. For example, hydrogenation of 4-methyldibenzothiophene yields methylbiphenyl and hydrogen sulfide (Reaction 13):

$$C_{13}H_{10}S + 3H_2 \rightarrow C_{13}H_{12} + H_2S \quad (13)$$

It is shown that a formation fluid saturated with sulfur-containing compounds, when reacting with hydrogen generated by deep geochemical processes, reduces the concentration of thiols, sulfides, disulfides, thiophenes, sulfoxides, and sulfones, while the concentration of hydrocarbons increases and hydrogen sulfide (H_2S) is produced.

4. DISCUSSION

It has been demonstrated that kerogen type is a determining factor in the component composition of formation fluids. Algal-type kerogen predominantly generates liquid hydrocarbons with low sulfur content but high nitrogen content. Marine kerogen is characterized by high sulfur content, which contributes to the formation of significant amounts of thiols, sulfides, and thiophenes. Humic (terrestrial) kerogen, on the contrary, generates mainly gas and aromatic hydrocarbons, with a minimal amount of sulfur-containing compounds but a high content of oxygen-containing components.

Pressure–temperature (thermobaric) conditions during catagenesis have a decisive influence on the

chemical transformations of organic matter. At 100–150 °C, the formation of alkanes, naphthenes, thiols, and sulfides dominates, as well as linear oxygen- and nitrogen-containing compounds. As temperature rises to 150–300 °C, aromatization and dehydrogenation occur, leading to an increased fraction of arenes, thiophenes, and complex nitrogenous compounds, while the content of oxygen-containing components decreases due to decarboxylation.

The mechanisms of formation of sulfur-containing compounds include thermolysis, radical recombination, cyclization, and aromatization. Thiols and sulfides form in the early stages of catagenesis by breaking weak C–S and S–S bonds. Thiophenes and their derivatives form at higher temperatures via cyclization and aromatization of sulfur-bearing fragments, which requires the presence of H_2S. Sulfoxides and sulfones typically form not in the catagenesis zone but during fluid migration toward the surface by oxidation of sulfides in the presence of oxygen or other oxidants.

Thermodynamic analysis based on Gibbs free energy indicates that the formation of thiols is a spontaneous process at all stages of catagenesis. The formation of thiophenes is thermodynamically possible at high temperatures and sufficient H_2S concentrations. The formation of sulfides, disulfides, sulfoxides, and sulfones is possible only in the presence of oxidizers, which suggests their generation predominantly during migration and accumulation in traps.

Hydrodesulfurization of sulfur-containing compounds through interaction with hydrogen introduced into the reservoir by deep geochemical processes leads to a reduction in the concentration of thiols, sulfides, disulfides, and thiophenes, accompanied by an increase in hydrocarbon content and the formation of hydrogen sulfide (H_2S). These reactions proceed with varying degrees: thiols are easily desulfurized, whereas thiophenes and polycyclic sulfur compounds are resistant and require severe conditions.

The complex interplay of geochemical factors—kerogen type, temperature, pressure, availability of hydrogen and oxidants—determines the final composition of oil. This allows the use of data on heteroatomic compounds (S, N, O) as biomarkers to reconstruct the conditions of oil formation and migration, as well as to assess the degree of catagenetic maturity of organic matter.

Discoveries of oil reservoirs in zones of extreme temperatures and pressures indicate the need to revise long-established views on the formation of accumulations both in high-organic (domanik) strata and on their role in the petroleum potential of sedimentary basins. It is evident that to reconstruct the conditions of hydrocarbon formation in specific clayey, siliceous-clayey high-organic strata, one must consider not only the burial and heating history, but also the influence of pressure, tectono-geodynamic processes, and the interplay of organic transformation processes with deep fluid mass transfer and the energy input of deep gases (hydrogen in particular).

The research also findings highlight the need to reconsider the deep «oil window» limit: at high pressures, oil may persist at depths of up to 7–8 km, especially in the presence of hydrogen. For instance, the formation of thiophenes becomes thermodynamically favorable at $T > 220$ °C and $P > 120$ MPa, corresponding to a depth of ~6.5 km with an average geothermal gradient of 35 °C/km.

Another critical factor for hydrocarbon accumulation at great and ultra-great depths is the preservation of reservoirs and the reservoir properties of rocks, which requires additional scientific research (42-44).

There has also been a growing application of machine learning and hybrid models to optimize thermodynamic calculations in recent studies (45).

5. CONCLUSION

Despite significant progress in understanding the processes of petroleum generation, existing geochemical methods and basin modeling have limited applicability at great depths (>5–6 km) under extremely high temperatures and pressures.

The obtained results show that the formation of thiols is thermodynamically favorable throughout all stages of catagenesis, whereas thiophenes and more complex sulfur-bearing structures form only in high-temperature zones with sufficient H_2S. Natural hydrodesulfurization reactions, confirmed by modeling, indicate that interaction with hydrogen from deep geological processes reduces the concentration of sulfur-containing components and increases the proportion of hydrocarbons in deep reservoir fluids.

Comparison of kerogen types and their temperature-dependent transformation pathways also shows that the distribution of heteroatomic (S, N, O) compounds can serve as an indicator of catagenetic maturity and deep reservoir conditions.

The novelty of the study lies in integrating thermodynamic equilibrium calculations with geochemical reaction mechanisms of heteroatomic compounds under ultra-high P–T conditions, which allows reconsideration of hydrocarbon stability limits at depths beyond 5–6 km.

Current methods for predicting petroleum systems must be used very cautiously when moving into depth ranges beyond 5–6 km. Only a combination of different approaches – thermodynamic, kinetic, and geophysical – and their mutual calibration will gradually reduce uncertainty and increase the reliability of predictions of the presence of oil and gas at the greatest depths.

Further research directions include:

- Development of experimental setups to simulate conditions of 300 °C / 150 MPa.
- Deeper integration of the influence from deep-seated fluid flows (H_2, CH_4) into thermodynamic models.
- Combination of AI and physics-based models for extrapolating hydrocarbon system properties.
- Expansion of databases on heavy fractions and heteroatomic compounds under extreme P–T conditions.

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Ethics Approval and Consent to Participate

This article does not involve any studies with human participants or animals performed by any of the authors. Therefore, ethics approval and consent to participate are not applicable.

Competing Interests

The author declares no financial or organizational conflicts of interest.

Data Availability

The data that support the findings of this study are available upon reasonable request.

Declaration of Generative AI and AI-assisted Technologies in the Writing Process

During the preparation of this manuscript, the author used ChatGPT exclusively for minor language editing and stylistic refinement to improve clarity and readability. The author carefully reviewed, revised, and approved the final content and takes full responsibility for the accuracy, integrity, and originality of the work.
The author declares that there are no known financial or organizational conflicts of interest that could have influenced the work reported in this paper.

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Persian Abstract

چکیده

کشف مخازن نفتی در اعماق زیاد و بسیار زیاد، بازنگری در مفاهیم موجود در مورد امکان تولید و حفظ هیدروکربن در شرایط فشار–دمای بسیار بالا را ضروری ساخته است. این کار، رویکردهای ژئوشیمیایی و روش‌های مدل‌سازی حوضه مورد استفاده برای پیش‌بینی تولید هیدروکربن در اعماق زیاد را تجزیه و تحلیل می‌کند. این کار تأثیر دما و فشارهای بالا، سرعت دفن، انتقال فاز و سایر عوامل را بر تشکیل و تخریب نفت و گاز بررسی می‌کند. تجزیه و تحلیل سیستم‌های هیدروکربنی عمیق انجام می‌شود و پتانسیل مدل‌سازی ترمودینامیکی ترکیبات تعادل سیال و نتایج آزمایش‌های مربوط به تبدیل نفت در شرایط فشار–دمای بالا در نظر گرفته می‌شود. یک رویکرد مدرن برای ارزیابی یک سازند با کربن آلی بالا (Domanik) ارائه می‌شود که امکان ارزیابی پتانسیل تولید هیدروکربن را فراهم می‌کند. دلایلی که روش‌های ژئوشیمیایی موجود و مدل‌سازی حوضه می‌توانند نتایج بی‌نتیجه‌ای برای فرآیندهای مشابه در اعماق زیاد تحت شرایط فشار–دمای شدید ارائه دهند، شناسایی می‌شوند. به طور خاص، منابع عدم قطعیت در انتقال فاز هیدروکربن، مرتبط با فقدان داده‌های تجربی برای کالیبراسیون مدل و محدودیت‌های مدل‌های ترمودینامیکی فراتر از محدوده‌های معتبر آنها، در میان سایر عوامل، مورد بحث قرار می‌گیرند.