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Perspective

Mechanisms of hydrocarbon generation from organic matters: Theories, experiments and simulations

Shuheng Du[1,2]*, Tao Hu[3,4]

[1]State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, P. R. China

[2]School of Engineering Science, University of Chinese Academy of Sciences, Beijing 100049, P. R. China

[3]State Key Laboratory of Petroleum Resources and Engineering, Beijing 102249, P. R. China

[4]College of Geosciences, China University of Petroleum (Beijing), Beijing 102249, P. R. China

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Abstract:
A comprehensive understanding of the characteristics and mechanisms underlying hydrocarbon generation from organic matter has emerged as a pivotal challenge in deciphering the "life mystery" of oil and gas, thereby guiding strategic planning for the global petroleum industry. The swift advancements in materials science, drilling engineering, computer technology, big data, and artificial intelligence have furnished robust methodologies and tools for research into organic hydrocarbon generation. This perspective offers an analysis and synthesis of three distinct research paradigms pertinent to organic hydrocarbon generation: Theoretical analysis, experimental exploration, and numerical simulation. These three research modalities probe the mechanisms of organic hydrocarbon generation across varied scales, with their findings mutually reinforcing and validating each other. This synergy provides invaluable insights that contribute to a holistic understanding of organic hydrocarbon generation, facilitating a comprehensive assessment of the potential of subterranean oil and gas resources.

1. Introduction

Petroleum geology, a significant branch of applied geology, primarily investigates the laws governing the generation, migration, and aggregation of oil and gas. Central to this field is the scientific issue of oil and gas generation, which holds paramount importance for both the theoretical framework of petroleum geology and the progression of the petroleum industry (Li et al., 2021). The precise origin of oil and gas remains a topic of ongoing debate. However, the "organic origin theory," which posits that hydrocarbons are formed by organic matters, has gained widespread acceptance due to the discovery of numerous oil and gas fields in global basins (Yang et al., 2023). Consequently, organic matter, exemplified by kerogen, is frequently termed as the "parental material" of oil and gas. Comprehensively understanding the characteristics and mechanisms of hydrocarbon generation from organic matters has become paramount in deciphering the "life mystery" associated with oil and gas, as well as guiding the strategic design of the global petroleum industry.

The rapid advancement of fields such as materials science, drilling engineering, computer technology, big data, and artificial intelligence has led to a tripartite approach in the study of organic matter hydrocarbon generation (Fig. 1): Theoretical analysis, experimental exploration, and numerical simulation. In recent years, researchers across various disciplines have delved into the enigma of organic matter hydrocarbon generation, employing the aforementioned three research paradigms. The findings from these studies are not only complementary but also mutually corroborative, offering valuable perspectives on unraveling the intricacies of organic matter hydrocarbon generation holistically and assessing the potential of subterranean oil and gas reserves.

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*Corresponding author.
E-mail address: dushuheng@imech.ac.cn (S. Du); thu@cup.edu.cn (T. Hu).

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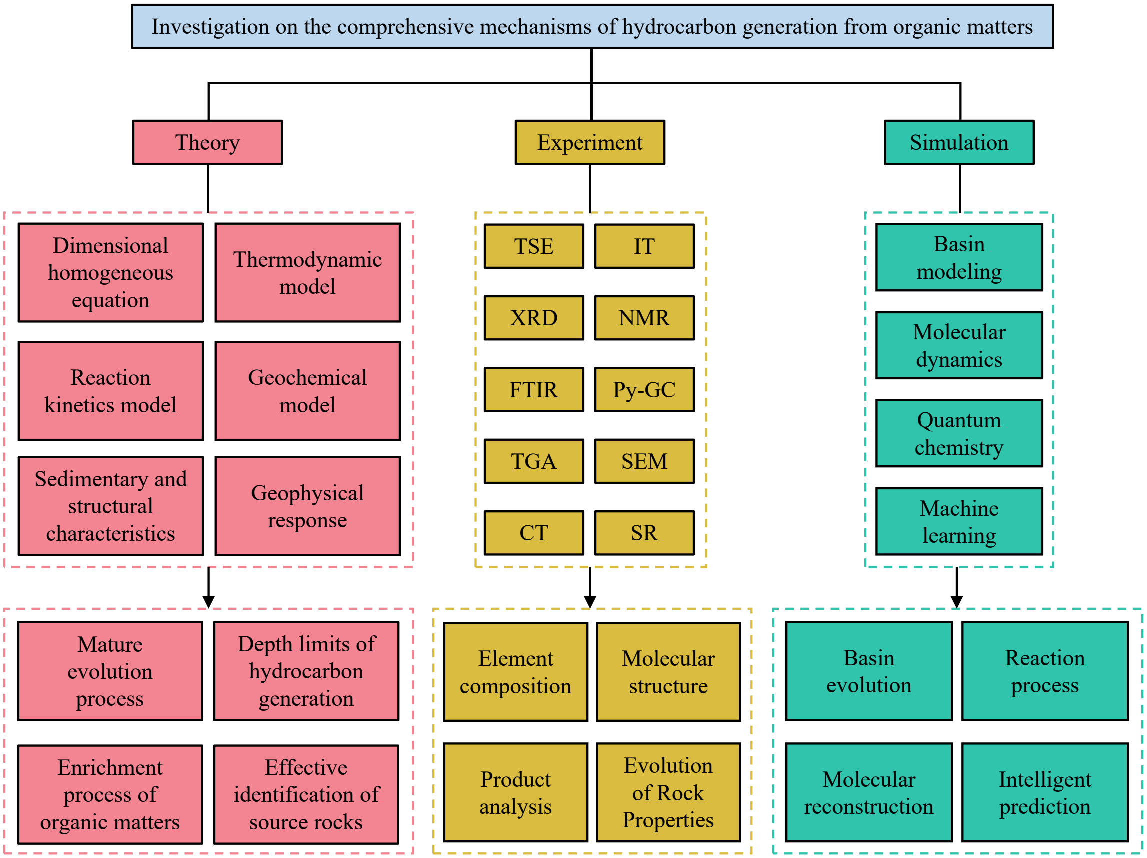

Fig. 1. Research paradigms of hydrocarbon generation from organic matters. (Note: "TSE", "IT" indicate "Thermal simulation experiment" and "Isotope tracking", respectively.)

2. Mechanisms of hydrocarbon generation from organic matters

At the macro-scale, the history of sediment burial, basin thermal history, tectonic evolution, organic matter maturation evolution, and hydrocarbon generation all exist in a continuous, complementary, and inseparable sequence. At the micro-scale, organic matter is composed of stable macromolecules with complex molecular structures, ultra-large molecular weights, numerous fatty branched chains, and low activation energy for hydrocarbon generation at the onset of burial. Through sedimentation and diagenesis, organic matter transitions into the hydrocarbon window, where its structure becomes simpler, molecular weight decreases, fatty branched chains diminish, and the activation energy for hydrocarbon generation increases. Thus, the entire process of hydrocarbon generation in organic matter can be viewed as a process of hydrogen redistribution and carbon ordering. The reconstruction of the actual organic matter molecular structure and hydrocarbon generation process using theory, experimentation, and simulation is of significant importance.

2.1 Theoretical analysis

The primary theoretical challenges in understanding the "life mystery"of oil and gas revolve around the upper and lower depth limits of hydrocarbon generation. The upper depth limit, or threshold, signifies the point at which kerogens commence producing significant amounts of hydrocarbons, indicating the inception of oil and gas production. Conversely, the lower limit, or death line, denotes the point where kerogens cease their activity and stop generating hydrocarbons, signifying the cessation of oil and gas production. A statistical empirical estimation formula proposed for the depth lower limit of organic matter hydrocarbon generation, drawing on extensive experimental data from the fields of oil and gas geochemistry and geothermal flow data (Pang et al., 2022). This was achieved by integrating trend analysis methods and two-dimensional linear fitting. A significant negative correlation between the depth lower limit of hydrocarbon generation and both the hydrogen index and geothermal flow was suggest. The concise estimation equations for the physical dimension matching of the "upper limit" and "lower limit" of hydrocarbon generation depth were developed by integrating mechanical and geological principles. Approximately 20% of global basins have the hydrocarbon generation lower depth limits exceeding 10,000 meters. The global maximum value of the lower depth limit of hydrocarbon generation is approximately 16,337 m (Du, 2021; Du et al., 2023). All these findings offer novel mechanical perspectives for elucidating the emergence and disappearance mechanisms of oil and gas.

Elucidating the enrichment law of organic matter is a pivotal theoretical endeavor for optimizing exploration efficiency

(Awan et al., 2020; Cao et al., 2023). The paleoproductivity, paleoenvironment and hydrothermal events of the Niutitang formation in western Hubei have shown that hydrothermal activity and sea level fluctuation controlled the redox conditions and paleoproductivity of seawater and ultimately controlled the organic matter accumulation of Niutitang formation (Niu et al., 2021).

The precise identification of stratigraphic sections associated with effective source rocks in shale constitutes a significant theoretical challenge for conducting oil and gas resource assessments. Two types of shale including dark laminated and grey massive shales in Bohai Bay Basin could be identified and it helps to confirm that oil and gas resources in the continental strata mainly come from the dark laminated shales with high organic carbon content (TOC>1.0%) and oil-prone kerogen. The results provide practical guidelines for conventional petroleum exploration and shale oil sweet spots prediction (Hu et al., 2022, 2024).

Biomarker compounds hold significant implications for sedimentological studies and source identification (Chen et al., 2017). As to the tricyclic terpanes in the Upper Paleozoic coal-measure source rocks in Ordos basin, the transformation of higher plants by microorganisms makes the hydrocarbon-forming parent material of type II coal-measure source rocks different from that of type I source rocks with original higher plants as hydrocarbon-generating parent materials (Lin et al., 2023).

2.2 Experimental exploration

Thermal simulation experiments offer a controlled experimental environment for researchers to systematically manipulate parameters such as temperature, pressure, and organic matter type. This facilitates an in-depth and direct investigation into the kinetics and thermodynamic properties of hydrocarbon generation by organic matter under varying conditions. Concerning the gold-tube pyrolysis of Eagle Ford Shale using miniature core plugs, the retardation effect of pressure on hydrocarbon generation and expulsion as well as pore evolution may provide a mechanism for the Type II kerogen-dominated oil-prone shales to become potential shale gas reservoirs (Shao et al., 2022a, 2022b). Meanwhile, the others discuss the anhydrous glass tube isothermal pyrolysis simulation for a crude oil and indicate that effluent pressure promotes the cracking of crude oil, increasing yields of C_1–C_5 saturates but inhibiting the generation of olefins (Shi et al., 2023).

The intricate physicochemical interactions between various liquids, exemplified by water, and rocks are termed water-rock interaction. Water-rock interaction significantly influences the production of oil and gas. The higher hydrogen fugacity may promote the hydrocarbon generation of low-maturity shale, and the yields of gaseous hydrocarbons and lighter components in product are significantly improved (Fang et al., 2022). Generally, the model of hydrocarbon generation is a function of temperature, hydrogen fugacity, proportions of organic functional groups and the corresponding reaction kinetics parameters (Wu et al., 2022). While hydrocarbon generation would be influenced by water-rock interaction, the validity requires further verification through in-depth drilling. These proposals are thus advocated for enhanced exploration in subsequent research endeavors.

It is important to note that as organic matter hydrocarbon generation progresses, there are corresponding changes in the pore structure of organic matter and the mechanical properties of rock. The nanoindentation method was utilized to investigate the changes in mechanical properties during hydrocarbon generation. The results showed that at similar pyrolysis temperatures, mechanical parameters of the hydrous pyrolysis product generally exhibit lower values compared to those of the anhydrous pyrolysis product (Yu et al., 2022; Liu et al., 2023) . The necessity for a comprehensive understanding of the law governing the variation of mechanical properties is evident, as it aids in accurately identifying the location and flow mechanism of oil and gas.

The *in-situ* transformation of shale serves as a crucial method for achieving low-maturity shale oil and gas exploitation. To accurately characterize the physicochemical process of this transformation, it is imperative to employ standard theoretical models in conjunction with experimental results. A new peak deconvolution method could be used to divide the multi-step reaction process of Nenjiang formation shale in Songliao basin to explain its *in-situ* conversion mechanism. The findings provide theoretical support for the development of *in-situ* heating conversion technology for medium-low maturity shale oil in the Songliao Nenjiang Formation (Zhao et al., 2018).

2.3 Simulative investigation

Geological and basin modeling have emerged as pivotal tools for optimizing exploration on a large scale. This process necessitates the provision of a substantial amount of valid experimental data or theoretical models to support it effectively. High-accuracy geological model could be established for simulating the generation and expulsion history of hydrocarbons in the Longtan Formation source rock in the Sichuan Basin (Zhang et al., 2022).

Molecular dynamics simulations of the changes in some special biomarker compounds during hydrocarbon genation process can often bring us new insights (Li et al., 2021). Five reaction pathways implicated in the initial pyrolysis of 4, 4, 8, 10-tetramethyl decalin: Three demethylation reactions (more likely to occur) and two ring-opening reactions (Chen et al., 2017).

Machine learning techniques exhibit robust capabilities for intricate problem analysis, adept at discerning hidden patterns within data and subsequently predicting unobserved scenarios. A prevalent challenge in the reconstruction of organic matter macromolecules is the suboptimal efficiency of traditional methods due to the complex origins, substantial molecular weights, and diverse functional groups of kerogen molecules. Consequently, machine learning emerges as a potential alternative for the efficient reconstruction of these molecular models. An intelligent high-throughput platform needs to be developed for kerogen construction utilizing ensemble learning, facilitating intelligent, high-throughput reverse reconstruction of molecular models based on empirical data (Kang et al., 2021). Building upon this foundation, the interplay between orbital hybridization, molecular structure, and maturity could be investigated by machine learning techniques. The crucial mechanism of structural changes during kerogen maturation is actually an increase in sp^2 hybridized atoms and a decrease in sp^3 hybridized atoms. This insight offers valuable theoretical groundwork for future research into the hydrocarbon generation potential of kerogens and the prediction of shale oil and gas production (Ma et al., 2022).

3. Conclusions

Hydrocarbon generation holds a pivotal role in petroleum geology. This issue is fundamentally multifaceted, spanning across various scales, and presents numerous scientific challenges that warrant exploration at each level. Addressing this issue necessitates a combination of theoretical, experimental, and simulative approaches, tailored to the specific nature of the issue.

1) From a theoretical standpoint, it is imperative to integrate principles of geology with multidisciplinary concepts such as mechanics and chemistry. The investigation into the upper and lower limits of hydrocarbon generation, the enrichment mechanisms of organic matter and conducting research on effective source rocks are essential. There should be a synergy between theoretical insights and laboratory experiments, coupled with logging data.
2) Regarding experimental exploration, the thermal simulation experiment is of direct relevance to oil and gas sweet spots exploration and development. Furthermore, future research should prioritize the application of mathematical statistical theory models to describe the experimental results of hydrocarbon generation, thereby achieving a harmonious integration of theory and experimentation.
3) Regarding numerical simulation, investigating the alteration characteristics of specific biomarker compounds during the hydrocarbon generation process through molecular dynamics simulation often yields novel insights. In forthcoming research, machine learning is emerging as a pivotal technique for efficiently reconstructing the molecular model of kerogens and elucidating the hydrocarbon generation mechanism of organic matter.

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Conflict of interest

The authors declare no competing interest.

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