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Perspective

Quantitative characterization and source tracing of fluids in shale oil and gas reservoirs: Progress and prospects

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Abstract:
Shale oil and gas are strategic resources for global energy structure transformation and national energy security. Shale reservoirs are characterized by well-developed nanoscale pores, extreme heterogeneity, the coexistence of multiphase fluids, and significant fluid-solid interactions. The accurate quantitative characterization of multiscale, multiphase fluids has become a core issue limiting the improvement of exploration and development benefits. Focusing on key scientific issues such as the quantitative characterization and source tracing of fluids in shale oil and gas reservoirs, this work systematically describes the relevant physical experimental techniques, numerical calculation methods and theoretical evaluation models, then summarizes the main research achievements and technological breakthroughs in the occurrence mechanisms of multiphase fluids, identification and quantitative evaluation techniques of multiphase fluids, temperature-pressure coupling evolution, and source tracing in shale reservoirs. Finally, future development priorities are projected from four directions: in-situ multiphase fluid content and distribution in reservoirs, the gas quantum physical adsorption model, the multi-field coupling dynamic evolution model, and cross-scale fluid source tracing. Through this structured approach, this work aims to provide solid theoretical and technical support for the evaluation of sweet spots and the efficient development of shale oil and gas.

1. Introduction

Due to the unique geological characteristics of shale reservoirs, our limited understanding of fluid occurrence and migration seriously restricts development efficiency and the full utilization of resource potential. Unlike those in conventional oil and gas reservoirs, shale fluids coexist as adsorbed, capillary-bound and free states in organic pores, inorganic pores and fractures. Traditional well logging, core analysis and numerical simulation cannot accurately quantify different-phase fluid compositions, distinguish multiphase distributions, or predict dynamic responses during development. Recently, experimental techniques including nuclear magnetic resonance (NMR), micro-nano CT, scanning electron microscopy, gas adsorption pore structure characterization, and geochemical tracing have further advanced. Moreover, molecular dynamics and multi-field coupling numerical simulations are now widely applied, providing key support for multiscale multiphase fluid characterization. Aimed at tackling the key challenge of fine fluid characterization in shale oil/gas reservoirs, this work systematically reviews frontier progress in multiphase fluid

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occurrence mechanisms, identification and quantitative evaluation techniques, temperature-pressure evolution, and fluid source tracing, in order to provide theoretical and technical support for sweet spot evaluation and the efficient development of shale oil and gas.

2. Occurrence mechanism and characterization of multiphase fluids

2.1 Shale oil

Shale oil exists primarily in free, adsorbed and dissolved states, with free oil constituting the currently recoverable portion. A series of methods for evaluating shale oil content have been derived, including stepwise pyrolysis, solvent sequential extraction, swelling experiments, molecular simulation, and NMR. Based on these methods, it is widely recognized that shale oil occurrence is governed by pore characteristics, temperature, pressure, and hydrocarbon type. Generally, oil forms multilayer adsorbates on pore surfaces, and the pore center accommodates free oil. Micropores are dominated by adsorbed oil, whereas larger pores contain a higher proportion of free oil (Zhang et al., 2023). Variations in the fluid properties and reservoir conditions determine the regional differences in these occurrence patterns. Because mineral composition and pore structure are inherently linked (Song et al., 2024; Song et al., 2026), clarifying their matching relationship across different reservoirs and quantitatively characterizing fluid-solid interactions within these mineral composition-pore structure units remain critical research directions for advancing the study of shale oil occurrence states.

2.2 Shale gas

Shale gas (mainly methane) occurs primarily as physically adsorbed gas on organic/clay surfaces, partly as free gas in pores/fractures, and rarely dissolved in kerogen/bitumen. Current research methods for shale gas include field desorption, isothermal adsorption experiments, and molecular simulation. Isothermal adsorption is the core technique for quantifying methane adsorption capacity, revealing the relevant mechanisms by regulating environmental (pressure, temperature, water content) and reservoir variables (composition, maturity, pore structure). To this end, selecting the right adsorption model is crucial; commonly used models include thermodynamic, kinetic and potential energy-based models, with the Langmuir model being the most widely used. New hypotheses, such as the quantum-physical adsorption model (Li and Cai, 2023), suggest that gravitational potential energy is quantized in confined nanoscale spaces, where potential energy determines spatial occupancy, and temperature affects adsorption probability, explaining the coexistence of adsorbed and free gas.

As shale gas exploration and development are advancing further, deep shale gas has become a key focus area. To this end, the accurate evaluation of in-situ gas content under deep conditions and the coexistence characteristics and transformation mechanisms of adsorbed gas and free gas during the evolution of complex geological conditions are key issues limiting the optimization of sweet spots and the calculation of reserves for deep shale gas.

2.3 Pore water in shale

Shale water exists in the states of structural, crystalline, adsorbed, and free water, with the latter two occupying pore spaces as pore water. Interactions between fluids and shale components are highly heterogeneous: inorganic minerals are generally hydrophilic, while organic matter is lipophilic, although surface functional groups can alter wettability (Cai et al., 2024). While pore water reduces storage space, it can enhance hydrocarbon mobility by weakening wall adsorption (acting as a lubricant). Water adsorption in pore networks is highly sensitive to relative humidity; as humidity increases, it transitions from monolayer to multilayer adsorption and, ultimately, to capillary condensation (Bai et al., 2020; Xing et al., 2025). This process is governed by both mineral composition and pore structure. Among the available thermodynamic models, the Dent multilayer model is preferred because it distinguishes between primary (strongly bound) and secondary (weakly bound) adsorption layers, thereby elucidating distinct pore-water states (Wang et al., 2019).

Compared with shale gas reservoirs, shale oil reservoirs have lower thermal maturity and a pore system dominated by inorganic minerals. Interlayer fractures within relatively high clay content provide a large specific surface area, significantly affecting water vapor adsorption (Zhang et al., 2024). Thus, unlike gas in hydrophobic organic pores, shale oil directly competes with water for hydrophilic or mixed-wet inorganic pores. Numerous NMR studies have confirmed that the space occupied by capillary-bound water matches that of adsorbed oil, while the space occupied by movable water matches that of capillary-bound oil (Xiang et al., 2024). Therefore, changes in pore water content inevitably alter the occurrence state of shale oil.

3. Identification and quantitative evaluation techniques of multiphase fluids

Shale reservoirs have complex pore-fracture systems containing oil, pore water and varying gases, where the occurrence of fluid varies with maturity and pore structure. Water saturation is key: pore water occupies hydrophilic pore surfaces and nanopores, competing with oil for space and restricting oil mobility. As a further complication, the gas-oil ratio also varies with maturity. Thus, clarifying the occurrence of oil-gas-water multiphase systems is essential for accurate resource and recovery assessment. Quantitative methods like stepwise pyrolysis and solvent extraction have limitations. Pyrolysis suffers from light hydrocarbon loss requiring correction (Lin et al., 2024), while extraction is time-consuming and cannot account for pore water (Wang et al., 2022a); basically, neither method considers water in the system.

NMR technology offers an efficient, non-destructive, and rapid evaluation on the oil-water components in pores, and reveals the occurrence of pore water and oil and their interactions. Combined with nitrogen adsorption and SEM, NMR characterizes the full-scale pore-size distribution. It effectively distinguishes kerogen, capillary-bound water, and adsorbed/capillary-bound/movable oil via two-dimensional rotational Gaussian functions (T_2 and T_1/T_2 values) (Wang et al., 2024). Fluid types are quantified by signal amplitudes, enabling the quantitative characterization of pore oil and water. However, fluid loss during sampling, transport and storage can cause analysis results to underestimate the actual content, making in-situ evaluation critical. A mature shale oil-water recovery process can restore pore fluid content, track fluid changes during the recovery stages, observe pore structure evolution, and clarify the influence of pore water on shale oil occurrence (Gao et al., 2025).

Medium-to-high maturity continental shale oil in China has a high gas-oil ratio (> 1000 m^3/m^3) that changes during production (Zhao et al., 2024), leading to the coexistence of oil-gas-water. Methane produces NMR signals under controlled conditions; signal amplitude depends on pressure, temperature, density, hydrogen index, and diffusion-relaxation effects, requiring calibration to gas content to distinguish adsorbed from free gas. Thus, NMR enables the joint quantitative evaluation of multiphase occurrence. Pore water resides in hydrophilic micropores and clay-related pores, affecting wettability, capillary pressure and oil storage space, while gas alters occurrence pressure and phase distribution. Existing research on microscopic characteristics and interaction mechanisms of oil-gas-water multiphase coexistence in shale remains scarce; systematically elucidating these areas is crucial for understanding seepage, improving resource evaluation, and enhancing oil recovery.

4. Temperature-pressure evolution and fluid source tracing

Temperature-pressure field evolution and fluid sources jointly control the whole process of generation, migration, enrichment, and preservation of unconventional oil and gas. With the development of technologies such as fluid inclusion analysis, laser Raman spectroscopy, micro-area in-situ isotope and basin simulation, supplemented by clumped isotope, noble gas tracing and diagenetic-chronological fine constraints (Huang et al., 2021; Wang et al., 2023), current research is advancing from static description to dynamic evolution, quantitative reconstruction and genetic tracing, with the new directions being multi-technology integration, multi-scale fusion and whole-process dynamic analysis.

Shale reservoirs generally undergo the process of burial subsidence-hydrocarbon generation overpressure-uplift pressure relief, where paleo-temperature-pressure reconstruction is key to understanding shale oil and gas generation and overpressure formation. Fluid inclusions are the most direct "geological records" of paleo-fluids. Laser Raman spectroscopy has realized the quantitative characterization of multiphase fluid inclusions in the methane system, confirming that shale is generally in an overpressured state at the maximum burial depth (Wang et al., 2022b). Paleopressure reconstruction methods based on phase behavior simulation software such as PVTsim have achieved a breakthrough from single-inclusion analysis to a systematic constraint of inclusions of different generations and compositions. The empirical prediction model for hydrocarbon fluid inclusions proposed by Ping et al. (2023) eliminates the need for complex iterative calculations and significantly improves the computational efficiency of paleo-temperature and paleo-pressure reconstruction.

Multi-method integration has become the mainstream trend in fluid source tracing. Isotope dating technology provides absolute time constraints for shale diagenesis and fluid evolution, enabling the precise determination of the timing of multi-stage fracture formation and fluid activity. Clumped isotopes, as "independent geothermometers", can trace the temperature and origin of fluids (Shen et al., 2021), while the isotopic compositions and abundances of noble gases can be used to constrain fluid sources, mass balance and phase interactions (Li et al., 2022). The combined application of vein petrography, fluid inclusion analysis, in-situ microscale isotopic, and trace element analysis enables the reconstruction of the compositional-temporal-temperature-pressure evolution of diagenetic fluids in shales.

5. Prospects

Significant progress has been made in the quantitative characterization of fluids in shale reservoirs. However, there are still core challenges in this field, such as multi-scale coupling, in-situ dynamics, high temperature and high pressure adaptation, and complex component distinction. In the future, systematic research should be focused on the following four major directions:

1) In-situ fluid quantitative characterization technology under reservoir conditions. Develop in-situ fluid quantitative evaluation models and methods adapted to downhole high-temperature and high-pressure environments, and realize the determination of multiphase fluid content and distribution under in-situ reservoir conditions.
2) Nanoscale fluid-rock interface interaction and quantum physical adsorption model. Deepen existing research on the interaction mechanism between nanoscale fluid molecules and mineral surfaces, and explore the influence mechanism of quantum effects on adsorption/desorption, diffusion and migration.
3) Multi-field coupling dynamic evolution model. Construct a multi-field coupling dynamic model that couples temperature, pressure, stress, and chemical action to accurately predict fluid migration and production laws during the whole development process.
4) Cross-scale fluid source tracing. The deep integration of microscopic inclusion analysis, macroscopic basin simulation and isotope chronology will be the core development direction. Cutting-edge technologies such as non-traditional/clumped isotopes, ultra-high precision micro-area in-situ analysis, artificial intelligence-driven basin simulation, and nano-microscale fluid inclusion analysis are important research directions in this regards. With continuous breakthroughs in theoretical innovation and experimental technology, the quantitative characterization of fluids in shale will certainly achieve leapfrog development, providing solid support for the efficient, green, and

sustainable production of global shale oil and gas.

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Conflicts of interest

The authors declare no competing interest.

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