

Research Progress on Heterogeneity Characterization Methods of Deep Coal-Rock Reservoirs

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Abstract

Against the backdrop of global energy structure optimization and the carbon peaking and carbon neutrality goals, deep coalbed methane (CBM) exploitation has become a strategic direction for China's CBM industry, yet the extreme and cryptic heterogeneity of deep coal-rock reservoirs severely restricts its efficient development. Accurate characterization of this heterogeneity is the key to optimizing deep CBM development plans and improving exploitation efficiency. This paper systematically reviews the 2020–2025 research progress of deep coal-rock reservoir heterogeneity characterization methods, elaborating on the multi-scale connotation and characteristics of the heterogeneity at both micro and macro levels. It comprehensively introduces experimental characterization technologies covering micro-nano pore and macro fracture-tectonic characterization, as well as the multi-scale technology fusion workflow. The paper also expounds on quantitative evaluation methods including fractal theory, geophysical and logging data inversion, and numerical simulation, and summarizes the application of machine learning and deep learning in intelligent characterization, which has become the core driving force of this research field. Finally, the paper points out the current key challenges such as difficult deep in-situ characterization, ineffective multi-scale information fusion, the "black box" problem of intelligent algorithms and scarce high-quality data, and proposes future research directions including developing in-situ dynamic 4D characterization technologies, fusing physical mechanisms with data-driven models, constructing deep coal rock big data and knowledge graphs, and applying digital twin technology. This study provides important guidance for the accurate characterization of deep coal-rock reservoir heterogeneity and the efficient exploitation of China's deep CBM resources.

Keywords

Deep Coal-Rock Reservoir; Heterogeneity Characterization; Multi-Scale Analysis; Experimental Characterization; Quantitative Evaluation; Machine Learning; In-Situ Characterization; Coalbed Methane Exploitation.

1. Introduction

1.1. Research Background and Significance

Driven by the sustained growth of global energy consumption and the strategic goals of carbon peaking and carbon neutrality, optimizing the energy structure and developing clean energy has become a worldwide consensus. Coalbed methane (CBM), an unconventional in-situ generated and stored natural gas in coal seams, boasts both energy and safety attributes. Its efficient exploitation and utilization not only effectively supplement the supply of conventional natural gas, but also markedly mitigate the risks of coal mine gas accidents and reduce greenhouse gas emissions, yielding tremendous economic, social and environmental benefits. China is endowed with abundant CBM resources, yet over 80% of these resources are hosted in deep coal seams at a burial depth exceeding 1000 meters. Thus, advancing towards deep

formations has become an inevitable choice and strategic direction for the development of China's CBM industry.

However, deep coal-rock reservoirs are not homogeneous ideal media but exhibit extremely strong heterogeneity, which refers to the spatial inhomogeneity of various reservoir rock properties. In comparison with shallow and middle-depth reservoirs, deep coal-rock reservoirs have undergone more intense diagenesis, tectonic movement and thermal evolution, resulting in more complex heterogeneous characteristics, specifically manifested as a sophisticated stress field, multi-scale pore-fracture systems, diverse coal body structures and intense tectonic reworking. [1] Such pronounced heterogeneity is the decisive factor governing the distribution of "sweet spots" in deep CBM reservoirs. It directly impacts the gas content, adsorption/desorption capacity and permeability of coal seams, as well as fracture propagation behavior under stimulation measures such as hydraulic fracturing. Therefore, accurate characterization and evaluation of the heterogeneity of deep coal-rock reservoirs are crucial for effectively predicting production capacity, optimizing well placement, and formulating rational drainage and stimulation schemes. Research on heterogeneity characterization methods for deep coal-rock reservoirs is not only a core component of geological theoretical research on deep CBM, but also a key technical support for the efficient, economical and safe exploitation of deep CBM resources, bearing great theoretical value and practical significance. [2-3]

1.2. Connotation and Specificity of Heterogeneity in Deep Coal-Rock Reservoirs

Heterogeneity in deep coal-rock reservoirs refers to systematic spatial variations in the key properties of reservoirs, which can be interpreted from the perspectives of different scales and genetic mechanisms. At the microscale, such heterogeneity is first reflected in the lithologic composition of coal rock: significant differences exist in the chemical structure, physical properties and pore development characteristics of different macerals (vitrinite, inertinite, exinite), leading to inhomogeneity in adsorption capacity and matrix permeability. Secondly, the inhomogeneity of pore structure also exerts a profound influence on reservoir quality: coal contains a large number of micropores (<2 nm), mesopores (2–50 nm) and macropores (>50 nm). The extremely irregular size, morphology, connectivity and spatial distribution of these pores form a complex pore network, and such heterogeneity directly governs gas storage and diffusion. In addition, mineral filling heterogeneity is another critical aspect: the types, contents and filling modes of primary and secondary minerals in coal vary considerably. These minerals can plug pores and fractures, thereby significantly impairing reservoir permeability.

At the macroscale, heterogeneity mainly refers to the inhomogeneity induced by coal body structure, sedimentary characteristics and tectonic processes at the core, logging and reservoir scales, primarily including coal body structure heterogeneity, bedding and rhythmic heterogeneity, and fracture system heterogeneity. Coal seams with different structural types exhibit substantial differences in mechanical properties and fracture system development, which are the primary causes of order-of-magnitude variations in permeability. Due to periodic changes in sedimentary environments within coal seams, interbedded structures of different coal lithotypes and partings are formed, resulting in vertical heterogeneity. The density, aperture, occurrence, extension length and filling degree of natural fractures (endogenic and exogenic fractures) vary drastically in space; these fractures serve as the main channels for gas seepage, and their spatial heterogeneity determines the anisotropy and spatial variability of reservoir permeability. Reservoir heterogeneity is also embodied in regional heterogeneity caused by sedimentary structures, which mainly refers to variations in reservoir parameters controlled by the distribution of sedimentary facies belts and regional tectonic frameworks at the block or basin scale.

In contrast to shallow reservoirs, the heterogeneity of deep coal-rock reservoirs is more "extreme" and "cryptic". The extremeness is manifested in the following aspects: the intrinsic characteristics, variation range and action intensity of heterogeneity in deep coal-rock reservoirs far surpass those of shallow reservoirs. High-rank coalification in deep formations leads to the extensive development of organic pores, yet the pore size distribution is more discrete, the proportion of nanoscale micropores surges with extremely uneven distribution. Meanwhile, high in-situ stress results in the extreme alternating distribution of microfractures in "closed zones" and "open zones", with the difference in pore-throat connectivity reaching several orders of magnitude. In addition, stress inhomogeneity of deep coal rock leads to extremely disparate degrees of pore compression in different micro-regions: pores in stress relaxation zones remain relatively well-developed, while micropores in stress concentration zones are compressed and throats are plugged, with the permeability difference ranging from 1 to 3 orders of magnitude.

The "crypticity" of heterogeneity in deep coal-rock reservoirs does not imply the absence of heterogeneity, but rather that its actual micro-heterogeneous characteristics are difficult to accurately identify and quantify due to the limitations of sampling and characterization technologies, as well as the superposition effect of multiple factors, leading to a significant deviation between surface characterization results and underground in-situ conditions.[4]

Observations at a single scale or analysis with a single technology have inherent limitations. Therefore, to accurately characterize the properties of deep coal-rock reservoirs, a comprehensive research approach integrating multi-scale and multi-technologies must be adopted to restore the real in-situ reservoir conditions to the greatest extent possible.

2. Experimental Characterization Technologies for Heterogeneity of Deep Coal-Rock Reservoirs

Experimental characterization constitutes the foundation for understanding the heterogeneity of deep coal-rock reservoirs. Direct or indirect measurements of coal-rock samples can yield structural and physical property information across different scales. Modern experimental technologies are capable of covering a wide scale range, from nanoscale molecular pores to centimeter-scale macro-fractures.

2.1. Research Background and Significance

Micro pores and fractures are the primary storage spaces and diffusion channels for CBM, and the heterogeneity of their structure directly determines the reservoir storage capacity and micro-scale migration characteristics.

2.1.1. Fluid Injection Method

Fluid injection methods are a class of classic approaches for inverting pore structure information based on the behavior of specific fluids injected into or adsorbed by porous media.

(1) High-pressure mercury intrusion porosimetry (MIP): This method is based on the principle that mercury, as a non-wetting fluid, can enter pore throats of different sizes only under different applied pressures. According to the Washburn equation, the higher the pressure, the smaller the radius of pore throats accessible to mercury. By recording the mercury intrusion pressure and volume to plot a correlation curve, parameters such as pore throat size distribution, porosity and specific surface area can be obtained. This method has a wide measurable pore size range of approximately 3 nm to 200 μm , making it an important means for characterizing the heterogeneity of mesopore and macropore structures in coal rock. However, MIP also has limitations: ultra-high pressure may compress and damage the pore structure of deep high-rank coal, leading to distorted measurement results; it only measures pore throats connected to the sample surface and cannot reflect information on closed pores;

the "ink bottle" effect may overestimate pore throat size; in addition, the toxicity of mercury poses hazards to the environment and operators. Nevertheless, high-pressure mercury intrusion porosimetry still holds important value in comparing the differences in pore throat structures among different coal-rock samples.

(2) Low-temperature gas adsorption method: This method involves the physical adsorption of gas molecules such as nitrogen (N_2) or carbon dioxide (CO_2) on the internal and external surfaces of coal samples at extremely low temperatures. By measuring the gas adsorption capacity under different relative pressures, an adsorption-desorption isotherm is plotted and analyzed using classic physical models. Low-temperature nitrogen adsorption (LT- N_2 GA) is mainly used to characterize mesopores and some macropores with a pore size range of 2–50 nm. The total specific surface area can be calculated using the Brunauer-Emmett-Teller (BET) model, and the pore volume and size distribution of mesopores can be analyzed using the Barrett-Joyner-Halenda (BJH) model. LT- N_2 GA is one of the core technologies for studying the heterogeneity of the gas diffusion channel network in coal. Low-pressure carbon dioxide adsorption (LP- CO_2 GA) can effectively enter micropores smaller than 2 nm at low temperatures due to the smaller molecular size of CO_2 and its higher saturated vapor pressure at room temperature, thus serving as a dedicated method for characterizing the heterogeneity of micropore structures in coal. Combined with density functional theory (DFT) or Monte Carlo (MC) simulation methods, the pore volume and size distribution of micropores can be accurately calculated, which is crucial for evaluating the gas adsorption and storage capacity of coal seams.[5-6]

High-pressure mercury intrusion, low-temperature nitrogen adsorption and low-temperature carbon dioxide adsorption are usually used in combination to obtain "full-pore size" distribution information from micropores and mesopores to macropores, thereby comprehensively evaluating the heterogeneity of micro pore structures.

2.1.2. Low-Field Nuclear Magnetic Resonance (LF-NMR)

This technology leverages the nuclear magnetic resonance phenomenon of hydrogen-containing fluids in a magnetic field. When fluid hydrogen nuclei in the sample are excited by radio frequency pulses, their relaxation behavior (mainly the transverse relaxation time T_2) is closely correlated with the size of the pores where they are located. In small pores, fluid molecules collide frequently with pore walls, resulting in a fast relaxation rate and a small T_2 value; conversely, a large T_2 value is observed in large pores. Pore size distribution can be inverted by analyzing the T_2 spectrum. This method enables rapid and non-destructive detection, and its core advantage is that it directly reflects the information of fluid-accessible pore space, which is more representative of the real reservoir fluid occurrence state than the measurement results in a dry state. By analyzing the peak shape, peak area and peak position of the T_2 spectrum, parameters such as porosity, pore size distribution and movable fluid saturation can be quantitatively evaluated, thereby revealing the heterogeneity of pore connectivity. In recent years, low-field nuclear magnetic resonance technology has also been widely applied to study the dynamic evolution of coal-rock pore structures during processes such as hydraulic fracturing and CO_2 injection.

2.1.3. High-Resolution Imaging Techniques

Different from the aforementioned indirect measurement methods, imaging techniques can directly observe the morphology, size and spatial relationship of pores and fractures, providing the most intuitive evidence of heterogeneity.

Scanning electron microscopy (SEM)/field emission scanning electron microscopy (FE-SEM) is a core conventional technology for the microscale characterization of coal rock. Its core principle is to scan the sample surface with a focused electron beam and generate images by collecting different types of signals such as secondary electrons and backscattered electrons. In

comparison with ordinary SEM, FE-SEM features higher spatial resolution and signal-to-noise ratio, enabling clearer capture of fine features. This technology can be used as the preferred method for observing the micro-morphology of coal rock, which can not only clearly display the morphology and development degree of various pores and microfractures at the micron to nanometer scale, but also directly present the filling state and distribution characteristics of minerals. After processing SEM images with professional image processing software, key parameters such as porosity, pore size distribution and shape factor can be quantitatively extracted, providing reliable data support for the quantitative evaluation of microscale heterogeneity.

Focused ion beam-scanning electron microscopy (FIB-SEM) is a revolutionary technology for 3D reconstruction of nanoscale pore networks. It integrates a focused ion beam (usually gallium ions) and an electron beam in the same vacuum chamber, and performs layer-by-layer nanoscale precise cutting of the sample with the ion beam. After each layer of cutting, the electron beam conducts high-resolution imaging of the newly exposed sample surface. Through a continuous "cut-view" cycle, a complete 3D image sequence of the micro-region of the sample can be obtained. Based on the 3D pore model reconstructed by this technology, key parameters that cannot be acquired by traditional 2D observation or indirect measurement methods can be obtained, which plays an irreplaceable role in in-depth analysis of the complex pore-throat connectivity and fluid transport characteristic heterogeneity inside the deep coal matrix.

Atomic force microscopy (AFM) and transmission electron microscopy (TEM) offer ultra-high spatial resolution at the atomic or molecular level. AFM accurately obtains the 3D morphology of the sample surface by detecting the weak interaction force between the probe tip and the sample surface, without the need for a vacuum environment and with minimal damage to the sample, and is often used to study the surface roughness of coal rock and the fine characteristics of nanoscale micropores. TEM requires thinning the sample to an ultra-thin state that is penetrable by electron beams, and is mainly used to observe the coal macromolecular structure, ultramicro pores and mineral crystal morphology. However, this technology involves a complex and cumbersome sample preparation process and is destructive to the sample, so it should be used with caution in the characterization of primary heterogeneity of deep coal rock.[7-8]

2.2. Characterization Technologies for Macro Fracture and Tectonic Characteristics

As the main seepage channels for deep CBM, the spatial heterogeneity of macro fractures directly determines the reservoir seepage capacity and anisotropic characteristics, being the core content of macroscale heterogeneity characterization. For the accurate characterization of macro fracture and tectonic characteristics, a variety of mature technical methods have been developed at present, mainly including computed tomography (CT) scanning technology, core observation and logging interpretation technology, which complement each other and enable the comprehensive capture of reservoir characteristics at the macroscale.

2.2.1. Computed Tomography (CT) Scanning

CT scanning technology realizes non-destructive characterization of the internal reservoir structure based on the difference in X-ray absorption capacity of different substances. Its core principle is as follows: an X-ray beam penetrates the sample and the transmission signal is received by a detector; combined with computer algorithms such as filtered back projection, a sequence of 2D tomographic images of the sample interior is reconstructed, and a 3D digital model is obtained after further stacking processing. Different gray values in the image correspond to substances with different densities, which can directly distinguish the coal matrix from other components.

In the characterization of macroscale heterogeneity of deep coal rock, Micro-CT (micro-focus CT) and industrial CT are the most widely used non-destructive testing tools, and their core

applications and analysis directions are mainly reflected in three aspects: first, 3D fracture network characterization, which can clearly identify and realize 3D visualization of natural and induced fractures inside coal rock, and quantitatively extract key parameters such as fracture length, aperture, occurrence, density and connectivity, providing data support for the evaluation of fracture heterogeneity; second, mineral distribution identification, which can accurately distinguish high-density minerals such as pyrite from low-density coal matrix relying on the difference in gray values, and clarify the blocking degree and spatial distribution characteristics of mineral filling on seepage channels; third, dynamic process monitoring, combining CT scanning technology with triaxial loading devices can realize real-time (4D) monitoring of the damage, fracture and seepage processes of coal rock under the action of different stresses, temperatures and fluids, and intuitively reveal the influence law of macroscale heterogeneity on the mechanical behavior and seepage path evolution of coal rock.

2.2.2. Core Observation and Logging Interpretation

Core observation is the most direct and traditional basic method in macroscale heterogeneity research. Through visual description and systematic photographing of complete cores obtained from drilling wells, core information such as coal body structure, coal lithotype, bedding development characteristics, natural fractures (focusing on recording their occurrence, density and filling material types) and parting development can be accurately acquired, providing a basic basis for subsequent reservoir evaluation and verification of other characterization technologies.

Logging technology is a key means to obtain continuous distribution information of underground reservoirs, which can effectively make up for the shortcomings of limited sampling in core observation and the inability to reflect the global characteristics of reservoirs. Among them, conventional logging curves are mainly used for coal seam identification, sublayer division, and calculation of basic reservoir parameters such as porosity and gas content; imaging logging can provide high-resolution borehole wall images, which can clearly show the distribution characteristics of fractures and bedding, and accurately determine their occurrence and aperture, being the core technology for evaluating the heterogeneity of fractures around wells. In recent years, the application of machine learning algorithms in the automatic interpretation of logging data has become increasingly widespread, which has effectively improved the efficiency and accuracy of lithology identification and fracture identification, providing a new path for the efficient characterization of macroscale heterogeneity.[9]

2.3. Multi-Scale Technology Fusion Characterization

The heterogeneity of deep coal-rock reservoirs features significant multi-scale superposition characteristics. From nanoscale micropores to meter-scale macro-fractures, heterogeneities at different scales are interrelated and mutually influential, and any single experimental technology has its fixed applicable scale range and limitations. For example, the gas adsorption method is adept at characterizing the nanoscale micropore structure but cannot provide pore spatial distribution information; SEM can clearly observe the micron-scale pore morphology but only obtain 2D surface characteristics; CT scanning can realize 3D fracture network reconstruction but its resolution is insufficient to capture the details of nano-micron scale micropores. Therefore, to comprehensively and accurately reveal the actual characteristics of the heterogeneity of deep coal-rock reservoirs, it is necessary to organically integrate characterization technologies of different scales and types to realize multi-dimensional and full-scale collaborative characterization.

At present, a typical multi-scale fusion characterization workflow mainly includes the following steps: first, low-pressure carbon dioxide adsorption (LP-CO₂GA) and low-temperature nitrogen adsorption (LT-N₂GA) are used to accurately characterize the structural parameters of

nanoscale micropores and mesopores inside the coal matrix, clarifying the basic characteristics of micro pores; second, FIB-SEM is used to perform nanoscale layer-by-layer cutting and imaging of representative micro-regions to complete micro-region 3D reconstruction, establish a digital core model from the nano to micron scale, and reveal the actual connectivity characteristics of pores and throats; third, Micro-CT is used to scan larger-sized core samples to obtain the 3D distribution law of pores and microfractures from the micron to millimeter scale, connecting microscale and macroscale characteristics; then, combined with the intuitive information from core observation and the continuous distribution data from imaging logging, the distribution characteristics of macro-fractures and bedding from the centimeter to meter scale are clarified to achieve global coverage at the macroscale; finally, through technical methods such as digital core modeling and geostatistics, data from different scales and sources are fused and upscaled, and a comprehensive geological model that can fully reflect the full-scale heterogeneity characteristics of deep coal-rock reservoirs is ultimately constructed, providing reliable support for the design of subsequent development plans.[10]

3. Quantitative Evaluation Methods for Heterogeneity of Deep Coal-Rock Reservoirs

After obtaining the basic structural and physical property data of deep coal-rock reservoirs through experimental characterization, scientific mathematical and physical methods need to be adopted for quantitative evaluation and characterization of reservoir heterogeneity. This process converts complex internal reservoir structure information into quantifiable parameters that can be directly used for reservoir numerical simulation, development plan design and engineering construction optimization, thus providing reliable theoretical and data support for the efficient exploitation of deep CBM. This chapter systematically expounds the quantitative evaluation methods for the heterogeneity of deep coal-rock reservoirs from three core dimensions: fractal theory, geophysical and logging data inversion, and numerical simulation.[11-12]

3.1. Fractal Theory and Its Application

The pore and fracture systems inside deep coal-rock reservoirs are characterized by disorder and irregular morphology, and such complex structures often exhibit statistical self-similarity at different scales, making them an ideal application object of fractal geometry theory. Breaking through the limitations of traditional geometry, fractal theory provides a powerful mathematical tool for quantitatively describing the "order in disorder" and structural complexity of reservoir pore-fracture systems, being one of the core methods for the quantitative evaluation of reservoir heterogeneity.

3.1.1. Basic Concepts of Fractal Theory

The core concept of fractal geometry is the fractal dimension (D). Different from traditional topological dimensions (0 for points, 1 for lines, 2 for planes, 3 for volumes), the fractal dimension can be a non-integer, and its core function is to measure the irregularity, fragmentation degree and the effectiveness of space occupation of fractals. For the pore structure of coal-rock reservoirs, a larger fractal dimension value usually indicates a rougher pore surface, a more complex internal structure and stronger microscale heterogeneity of the reservoir; for fracture networks, a larger fractal dimension means a more fully developed and densely distributed fracture network and more significant macroscale heterogeneity of the reservoir.

3.1.2. Calculation Methods of Fractal Dimension

There are various calculation methods for the fractal dimension, which mainly depend on the source of the basic data used. At present, in the research of deep coal-rock reservoirs, they are

mainly divided into two categories: calculation methods based on fluid injection data and calculation methods based on image analysis.

Calculation methods based on fluid injection data mainly carry out fractal dimension calculation relying on characteristic parameters obtained from fluid injection experiments, with two commonly used methods:

One is the Frenkel-Halsey-Hill (FHH) model, which is mainly applied to the analysis of low-temperature nitrogen adsorption experimental data. Its core principle is to describe the power-law relationship between the adsorption layer thickness and relative pressure. The fractal dimension D related to pore surface roughness can be obtained by logarithmic fitting of the adsorption isotherm data, and this method mainly reflects the heterogeneity characteristics of the mesopore-macropore surface.

The other is the thermodynamic model, which is based on high-pressure mercury intrusion (MIP) experimental data. By establishing a quantitative relationship between the injection work and the pore surface area, the fractal dimension that can reflect the complexity of the pore structure is calculated, which can effectively characterize the heterogeneity differences of the pore structure in different pore size intervals.

Calculation methods based on image analysis take microscale or macroscale reservoir images as core data, among which the box-counting method is the most widely used and intuitive fractal dimension calculation method. Its basic principle is as follows: square (for 2D images) or cubic (for 3D images) grids of different sizes are used to cover the binarized pore or fracture images, and the number of boxes required for each coverage is counted; since there is an obvious power-law relationship between the number of boxes and the box size, the fractal dimension is calculated by linearly fitting the data in a double logarithmic coordinate system to obtain the slope of the fitting straight line. This method has strong applicability and can be widely used in the fractal analysis of various pore-fracture images such as SEM and CT images.

3.1.3. Application of Fractal Dimension in Heterogeneity Characterization

As a concise and efficient quantifiable parameter, the fractal dimension is widely used in the quantitative evaluation of the heterogeneity of deep coal-rock reservoirs. Relevant studies have shown that there are significant differences in the fractal dimensions of pore and fracture systems of coal rocks formed under different coal ranks, different coal-rock components and different tectonic environments, and the strength of reservoir heterogeneity can be intuitively reflected through the numerical differences of fractal dimensions. For example, tectonically deformed coal is subjected to intense tectonic stress, resulting in severe fragmentation of the pore structure and more complex morphology, and its fractal dimension is usually significantly higher than that of primary structure coal. Based on this, the degree of tectonic reworking and the strength of microscale heterogeneity of coal rock can be quickly judged.

With the deepening of research, scholars have found that the pore structure of coal-rock reservoirs does not follow a single fractal law but exhibits significant multifractal characteristics. This means that different pore size ranges inside coal rock may follow different fractal laws, corresponding to different fractal dimensions. By calculating the multifractal spectrum, the inhomogeneity of pore distribution at different scales can be depicted more finely, thereby revealing the reservoir heterogeneity characteristics more comprehensively and accurately. For example, some studies have calculated the fractal dimensions of the adsorption stage and capillary condensation stage in sections using low-temperature nitrogen adsorption data to characterize the heterogeneity of the pore surface and pore structure respectively, and found that the response laws of the fractal dimensions in the two stages to coal rank are significantly different, providing a new perspective for in-depth analysis of the formation mechanism of reservoir heterogeneity.[13]

3.2. Geophysical and Logging Data Inversion

Most of the aforementioned experimental analysis and fractal theory calculations are carried out based on small-sized core samples, which can only reflect the local heterogeneity characteristics of the samples and are difficult to realize the comprehensive evaluation of reservoir-scale (interwell and regional scale) heterogeneity. Therefore, to accurately depict the global heterogeneity distribution law of reservoirs, it is necessary to rely on geophysical and logging technologies capable of large-scale detection, and realize the spatial expansion and quantitative characterization of reservoir parameters through data inversion and modeling.

Seismic attribute analysis and inversion are the core technologies for characterizing reservoir heterogeneity at the regional scale, known as the "wide-angle lens" for regional heterogeneity evaluation. Its core idea is as follows: regional seismic data are obtained through 3D seismic exploration, and various seismic attributes such as amplitude, frequency, coherence and curvature are extracted; combined with geological background analysis, the distribution characteristics of macro structures such as faults and folds can be effectively identified, and the main controlling factors of macroscale heterogeneity can be clarified; on this basis, using prestack seismic inversion technologies and establishing a seismic response model combined with core experimental data, the spatial distribution prediction of key reservoir parameters such as coal seam thickness, gas content, porosity and fracture density can be realized, thereby delineating reservoir "sweet spots" and providing a basis for the deployment of development well patterns. For example, based on the seismic response model and AVO (Amplitude Versus Offset) simulation, combined with machine learning algorithms to optimize the inversion process, the prediction accuracy of the lateral variation of coal seam thickness can be significantly improved, and the reservoir heterogeneity at the regional scale can be effectively characterized.

Logging-constrained geostatistical modeling is mainly used to solve the problem of interwell reservoir information gaps and realize the refined spatial characterization of reservoir parameters. Logging data have the advantage of high vertical resolution and can accurately obtain the variation characteristics of reservoir parameters in the vertical direction of a single well, but there are obvious information gaps between wells; geostatistical methods are classic means for predicting the spatial distribution of reservoir parameters in unknown areas using known well point data, whose core is to quantify the spatial correlation and variability of reservoir parameters by establishing variograms. In practical applications, based on logging data, with seismic inversion results as soft constraints and combined with geological laws, 3D geological models of porosity, permeability, coal lithofacies distribution, etc., that conform to actual geological conditions can be generated. Such models can intuitively and quantitatively display the spatial heterogeneity characteristics of reservoirs, being the core foundation for subsequent reservoir numerical simulation and development plan optimization. [14-15]

3.3. Numerical Simulation Methods

On the basis of experimental analysis and 3D geological modeling, numerical simulation methods simulate dynamic processes such as fluid flow and rock mechanical changes inside reservoirs by solving various mathematical and physical equations, belonging to a kind of "computational experiment" method. This method can effectively connect reservoir heterogeneity characterization with engineering applications, and has unique advantages in understanding how heterogeneity affects reservoir dynamic evolution and predicting development effects, being an important means for the quantitative evaluation and engineering application of the heterogeneity of deep coal-rock reservoirs.

Seepage simulation is one of the core applications of numerical simulation, and its core process is as follows: based on a 3D geological model containing reservoir heterogeneity characteristics, combined with reservoir fluid physical property parameters, a seepage mathematical model is

established to simulate the pressure drop, gas production and water-gas distribution laws inside the reservoir under different development plans. By comparing and analyzing the simulation results with field actual production data, the heterogeneity parameters in the geological model can be continuously corrected, a process known as "history matching"; the geological model after multiple history matching can more accurately reflect the real heterogeneity characteristics of the reservoir, providing reliable support for the optimization and adjustment of development plans.

Geomechanical simulation is mainly aimed at the particularity of the high in-situ stress environment of deep coal seams, focusing on the study of the coupling effect (fluid-solid coupling) between fluid flow and rock mechanical behavior, and is a key supplement to the heterogeneity evaluation of deep coal-rock reservoirs. Its core function is to study the distribution and variation law of effective stress inside the reservoir during CBM drainage and pressure reduction or hydraulic fracturing and pressure increase through numerical simulation, and how such stress changes lead to the opening, closing or expansion of natural fractures, thereby causing the dynamic evolution of the reservoir permeability field. This simulation result is crucial for understanding and predicting the production behavior of deep CBM, especially the dynamic changes of reservoir permeability. For example, through geomechanical simulation, it can be clearly shown how the heterogeneous distribution of natural fractures guides and interferes with the propagation path of artificial fractures during hydraulic fracturing, thereby forming a complex fracture network, providing a theoretical basis for optimizing hydraulic fracturing technology and improving stimulation efficiency.[16-17]

4. New Intelligent Characterization Methods: Application of Machine Learning and Deep Learning

With the advent of the big data era, traditional heterogeneity characterization methods relying on expert experience and simplified physical models are struggling to process high-dimensional, massive and multi-source heterogeneous geological data. As the core technologies of artificial intelligence, machine learning (ML) and deep learning (DL) provide new ideas for reservoir heterogeneity characterization with their strong nonlinear mapping ability and the advantage of automatically learning features from data.[18]

4.1. Rise of Machine Learning in Heterogeneity Characterization

The geological system is essentially an extremely complex nonlinear system, and reservoir heterogeneity is the result of the joint action of various geological factors (sedimentation, diagenesis, tectonics, etc.) over a long time scale. Its internal laws are often difficult to describe with simple mathematical formulas. Machine learning, especially deep learning algorithms, can construct deep and complex neural networks that can theoretically approximate any complex nonlinear function, making them highly suitable for solving intractable problems in geological science.

Compared with traditional statistical methods, machine learning has the following advantages: Data-driven: The model directly learns laws from data, reducing the dependence on a priori physical models and excessive assumptions. High-dimensional data processing capability: It can process dozens or even hundreds of features simultaneously and discover the hidden complex relationships between them. Strong generalization ability: With sufficient training data, the trained model can make accurate predictions on new and unseen data with good adaptability. Automatic feature extraction: Especially convolutional neural networks (CNN) in deep learning can automatically learn and extract the most effective features from raw data, avoiding tedious and subjective manual feature engineering.

4.2. Intelligent Lithology Identification and Reservoir Parameter Prediction Based on Logging and Seismic Data

Logging and seismic data are the primary data sources reflecting the underground reservoir heterogeneity. Intelligent interpretation of these data using machine learning is one of the most widely used and mature research directions at present.

4.2.1. Algorithmic Models and Applications

Commonly used algorithms: In this field, there are both classic machine learning algorithms such as support vector machine (SVM), random forest (RF), XGBoost and artificial neural network (ANN), and more complex deep learning models such as long short-term memory (LSTM) network, which is particularly suitable for processing logging data with sequence characteristics.

Intelligent lithology identification: Traditional lithology identification relies on logging cross-plots and expert experience, with strong subjectivity and low efficiency. Using machine learning, various logging curves can be used as input features, and the lithology results obtained from core analysis as labels to train a classification model. For example, some studies have used a variety of algorithms including decision tree, random forest, extreme gradient boosting and Extra Trees to identify the lithology of deep coal seams, and the results show that the Extra Trees algorithm performs the best in multiple evaluation indicators such as F1 score, precision, recall and MCC value. This enables the rapid, accurate and automatic identification of lithologies such as coal, sandstone, mudstone and partings.

Quantitative prediction of reservoir parameters: Key reservoir parameters such as porosity, permeability and gas content can usually only be obtained through core analysis, with high cost and discrete data points. Machine learning can establish a nonlinear mapping relationship from easily obtainable logging and seismic data to these key parameters. For example, models such as SVM, ANN and XGBoost can be used to predict the gas content or permeability of coal seams with logging curves as input, making it possible to obtain continuous reservoir parameter profiles and providing key data for refined reservoir evaluation.

4.2.2. Data-Driven and Model Construction

A typical intelligent prediction model construction workflow includes the following steps:

- (1) Data preparation: Collect and integrate logging data, core analysis data, seismic data, etc., and perform data cleaning, denoising and standardization.
- (2) Feature engineering: Select logging curves or seismic attributes that are most sensitive to the target variable as the input features of the model. Feature importance analysis is a key step, which can help understand which geological factors contribute the most to the prediction results.
- (3) Model selection and training: Select an appropriate machine learning model according to the problem type (classification or regression) and data characteristics.
- (4) Hyperparameter tuning: Use methods such as grid search, random search or Bayesian optimization combined with K-fold cross-validation to find the optimal hyperparameter combination of the model to prevent overfitting and improve the generalization ability of the model.
- (5) Model evaluation and deployment: Evaluate the performance of the model on an independent test set, and apply it to new wells or work areas to realize the intelligent prediction of heterogeneity.[19]

4.3. Quantitative Characterization of Micro Heterogeneity based on Image Analysis

Microscale images of coal rock such as SEM and CT images contain abundant heterogeneity information, but traditional manual or semi-automatic image analysis methods are inefficient and poor in repeatability. Deep learning, especially convolutional neural networks (CNN), has achieved great success in the field of image recognition and segmentation, providing a revolutionary tool for the high-throughput quantitative characterization of microscale heterogeneity.

Intelligent image segmentation: A CNN model can be trained to automatically identify and segment different phases in the image, such as coal matrix, pores/fractures and different types of minerals. In comparison with traditional threshold-based segmentation methods, deep learning models can learn more complex texture and contextual features, with more accurate segmentation results and stronger robustness.

High-throughput parameter extraction: Once the accurate segmentation of the image is completed, various quantitative parameters such as porosity, pore size distribution, fracture density, fractal dimension and mineral content can be calculated in batches and automatically. This makes it possible to conduct statistical analysis of a large number of microscale images, thereby enabling a more reliable evaluation of microscale heterogeneity and its spatial variability.

4.4. Intelligent Fusion of Multi-Scale Data

The ultimate goal of reservoir heterogeneity characterization is to establish a multi-scale and high-precision 3D geological model that can fuse all available information. This is a typical data fusion problem involving the effective integration of point data (core), line data (logging), surface data (profile) and volume data (seismic).

Deep learning provides new solutions for multi-scale data fusion. Specific neural network architectures can be designed, such as multi-input channel networks, which receive data from different sources as input simultaneously. Through feature fusion layers inside the network, the inherent correlations between these different types of data are learned, and finally a more accurate prediction result consistent with geological reality is output. This end-to-end learning method avoids information loss and error accumulation that may occur in the traditional multi-step and fragmented fusion process, being a cutting-edge direction for realizing truly intelligent data fusion.

5. Research Challenges and Future Prospects

Although significant progress has been made in the heterogeneity characterization methods of deep coal-rock reservoirs, especially in terms of multi-scale analysis and intellectualization, there are still many severe challenges to be addressed. At the same time, the continuous emergence of new technologies also points out the direction for future research.[20-22]

5.1. Main Challenges Faced by Current Research

High difficulty in deep in-situ characterization: At present, most experimental characterizations are carried out on cores taken to the surface under normal temperature and pressure, which leads to the release of internal stress of the cores and irreversible changes in the pore and fracture structure, failing to fully reflect their in-situ state under high temperature, high pressure and high in-situ stress in deep formations. The development of technologies and equipment capable of measuring under deep in-situ conditions is a major technical bottleneck faced at present.

Challenges in effective fusion and upscaling of multi-scale information: How to seamlessly connect and transfer information of data with different scales and physical meanings, from nanoscale pores (FIB-SEM) and micron-scale fractures (Micro-CT) to meter-scale structures (logging, seismic), is a huge scientific challenge. The physical laws and mathematical models of the upscaling process from microscale mechanisms to macroscale responses are still not completely clear, which is the key factor restricting the accuracy of refined reservoir simulation.

"Black box" problem and geological interpretability of intelligent algorithms: Although machine learning models exhibit excellent prediction performance, their complex internal working mechanisms are often like a "black box", making it difficult to explain the specific reasons for a particular prediction. This conflicts with the geological research paradigm that emphasizes causal relationships and physical mechanisms. How to enhance the geological interpretability of models, such as developing "physics-informed neural networks (PINN)" or "science-informed machine learning", and integrating geological laws into the model training process as constraints, is the key to improving the reliability and application value of models.

Scarcity of high-quality training data sets: Machine learning is data-driven, and the performance of the model is highly dependent on the quantity and quality of training data. The exploration and development cost of deep coal seams is high, and the amount of data from coring and analytical testing is relatively limited, especially in the new area exploration stage. Data scarcity seriously restricts the training and application of complex deep learning models. How to use technologies such as few-shot learning, transfer learning and data augmentation to address the challenge of insufficient data is an urgent problem to be solved.[23]

5.2. Prospects for Future Research Directions

Development of in-situ, dynamic and four-dimensional (4D) characterization technologies: The focus of future research should shift from static characterization to dynamic characterization. By developing high temperature and pressure resistant sensors and experimental systems, combined with technologies such as CT and NMR, real-time (the fourth dimension: time) monitoring and characterization of the dynamic evolution process of pore-fracture structure, stress field and seepage field of deep coal rock under real reservoir conditions during engineering activities such as mining, gas injection and fracturing can be realized.

Deepening the fusion of physical mechanisms and data-driven approaches: Pure data-driven models and pure physical models have their own advantages and disadvantages. The future trend is to construct "hybrid models" that deeply integrate the two. For example, using physical simulation to generate a large amount of high-quality "virtual data" to expand the training set and make up for the lack of real data; or adding control equations as regularization terms to the loss function of neural networks, so that the prediction results of the model not only fit the data but also do not violate the basic physical laws, thereby improving the generalization ability and interpretability of the model.

Construction of big data and knowledge graph for deep coal rock: Integrate all multi-source heterogeneous data related to deep coal rock in the region to build a standardized and shareable big data platform for deep coal rock. On this basis, use natural language processing and graph database technologies to construct a knowledge graph in the field of deep coal rock, connecting unstructured knowledge with structured data, and laying a foundation for higher-level artificial intelligence applications.

Digital twin technology for "transparent geological body": Digital twin is the ultimate form of future reservoir management. It aims to create a virtual digital model that is real-time synchronized, mutually mapped and dynamically interactive with the physical reservoir. This model will integrate all multi-scale and multi-physical field characterization data and models, can real-time receive and assimilate production dynamic data, realize accurate prediction of reservoir state, simulation and optimization of production plans and early warning of potential

risks. The ultimate goal is to realize the "transparent" management of the "black box" of deep coal-rock reservoirs and maximize the recovery efficiency of deep CBM.[24-25]

6. Conclusion

The strong heterogeneity of deep coal-rock reservoirs is the core problem governing the distribution of their "sweet spots" and development benefits. This paper systematically expounds the research progress of characterization methods for this problem in recent years, especially from 2020 to 2025.

In terms of characterization scale, the research has shifted from focusing on a single scale to full-scale comprehensive characterization covering the "nano-micron-centimeter-meter" range. It has become an industry consensus and research mainstream to organically integrate technologies such as gas adsorption, mercury intrusion, nuclear magnetic resonance, high-resolution imaging, CT scanning and logging-seismic to construct a comprehensive understanding of reservoirs.

In terms of evaluation methods, the research has evolved from qualitative description to refined quantitative characterization. Mathematical tools represented by fractal theory provide an effective way to describe the complexity of pore-fracture systems, while 3D geological modeling based on geostatistics and numerical simulation realizes the visualization of heterogeneity in space and the analysis of dynamic evolution.

In terms of technical means, artificial intelligence technologies represented by machine learning and deep learning are penetrating into all links of heterogeneity characterization with unprecedented depth and breadth. From the intelligent interpretation of logging and seismic data to the automatic analysis of microscale images and the intelligent fusion of multi-source heterogeneous data, intelligent characterization not only greatly improves the efficiency and accuracy, but also reveals complex laws that are difficult to be found by traditional methods, becoming the core driving force for the development of this field.

Despite significant progress, challenges such as deep in-situ characterization, multi-scale information fusion, interpretability of intelligent algorithms and data scarcity remain severe. Future research needs to face the real deep formation environment and focus on the development of in-situ and dynamic 4D characterization technologies; commit to the deep fusion of data-driven machine learning models and classic physical mechanism models to learn from each other's strengths.

In summary, the depth of understanding of the heterogeneity of deep coal-rock reservoirs determines the scope of deep CBM development. Only through comprehensive research with interdisciplinary integration, multi-technology fusion, and dual driving of data and mechanisms can the heterogeneity characteristics of deep coal-rock reservoirs be truly restored and revealed, providing a solid scientific theory and technical guarantee for the safe, efficient and green exploitation of China's deep CBM resources.

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