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Comparison of Monofractal and Multifractal Methods in Characterizing Coal Pore Structures

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Abstract

Coal pore structures commonly exhibit significant heterogeneity, and fractal theory provides an effective tool for the quantitative characterization of such complex structures. Regarding multi-scale pore data acquired by CO_2 adsorption (micropores), N_2 adsorption (mesopores), and mercury intrusion porosimetry (macropores), monofractal and multifractal methods differ fundamentally in their computational principles and characterization approaches.This review discusses three classic models for monofractal dimension: the Sierpinski model based on CO2 adsorption data, the Frenkel–Halsey–Hill (FHH) model based on N_2 adsorption data, and the Menger sponge model based on mercury intrusion porosimetry (MIP) data. It also introduces the calculation methods for multifractal spectral parameters derived from the box-counting method, including the generalized dimension spectrum D(q), the multifractal singularity spectrum f(α), and the spectral width Δα. On this basis, a systematic comparison of the two approaches is conducted from multiple perspectives. The monofractal dimension quantifies the overall average complexity of coal pore structures as a single scalar value, offering computational simplicity and high efficiency, which renders it suitable for rapid screening of large sample sets and global evaluation of pore complexity. In contrast, the multifractal approach enables a detailed characterization of pore size distribution heterogeneity across different scale intervals and local domains, and is particularly well-suited for high-resolution microstructural analysis of strongly heterogeneous samples, such as tectonically deformed coal. This study provides a theoretical foundation for the rational selection of fractal methods in the characterization of coal reservoir pore structures.

Keywords

Coal Pores; Fractal Dimension; Monofractal; Multifractal

1. Introduction

Coal reservoir pore structures directly control the adsorption, desorption, seepage, and production processes of coalbed methane, and thus constitute a core research subject for coalbed methane geological evaluation and gas disaster prevention[1].Pores in coal exhibit typical multi-scale, heterogeneous, and irregular distribution characteristics ranging from nanoscale micropores to microfractures. Conventional parameters such as pore size, pore volume, and specific surface area are insufficient to fully capture this complex architecture. As a mathematical tool for quantitatively describing the complexity of irregular geometries, fractal dimension provides an effective means for the detailed characterization of coal reservoir pore structures[2].Based on differences in characterization dimensions, fractal dimension can be categorized into monofractal and multifractal types.

Current studies have largely applied monofractal or multifractal methods independently, and systematic comparisons between the two approaches in terms of computational models, information granularity, and applicable scenarios remain insufficient. Focusing on CO_2 adsorption, N_2 adsorption, and mercury intrusion porosimetry data, this paper reviews three classical monofractal models (Sierpinski, FHH and Menger) and the calculation methods for multifractal spectral parameters, followed by a multi-perspective comparison of the two approaches. This study aims to provide a reference for the rational selection of fractal methods in the characterization of coal pore structures.

2. Fractal Characterization Methods

Before systematically introducing each fractal model, it is necessary to clarify their valid intervals and applicable scopes. The monofractal dimensions derived from CO_2 adsorption, N_2 adsorption, and mercury intrusion porosimetry (MIP) data all represent fractal characterizations of the three-dimensional pore structure of coal, with a theoretical valid interval of 2-3. The closer the value is to 3, the more complex and heterogeneous the pore structure. It should be noted that the three models differ in their computational principles and underlying assumptions; therefore, direct comparison of the absolute monofractal dimension values across different models is not advisable. In contrast to the monofractal approach, which outputs only a single overall average value, the multifractal method, through continuous functions such as the generalized dimension spectrum $D(q)$and the singularity spectrum $f(\alpha)$, can finely characterize the differentiated features of pore structures across different scale intervals and local regions, and is particularly suitable for in-depth analysis of strongly heterogeneous coal samples. The following sections will introduce the two types of methods, respectively.

2.1. Monofractal

2.1.1. Low-Temperature Carbon Dioxide Adsorption Method

Basic Principle:The low-temperature CO_2 adsorption method is based on the principle of physical gas adsorption. By measuring the CO_2 adsorption isotherm of coal under constant temperature conditions (typically 273.15 K), the micropore structure is characterized. As the kinetic diameter of CO_2 molecules is smaller than that of commonly used adsorbates such as N_2, CO_2 can more effectively access ultra-micropores that N_2 molecules are unable to penetrate. This method provides key parameters including micropore specific surface area, pore volume, and pore size distribution, with an effective detection range of approximately 0.3-2 nm. It is therefore an ideal technique for accurately characterizing the distribution of micropores (<2 nm) and ultra-micropores (<1 nm) in coal.

Fractal Model:The calculation equation of the Sierpinski model is as follows[3]:

$$Ln(V) = Lna + (3 - D_s)Ln(P - P_t)$$

Where：V is the mercury intrusion volume (mL/g),P is the pressure (MPa),Ptis the threshold pressure (MPa), and K is the slope of the double logarithmic plot of lnV versus ln(P−Pt). The fractal dimension Ds is then calculated as Ds=3−K.

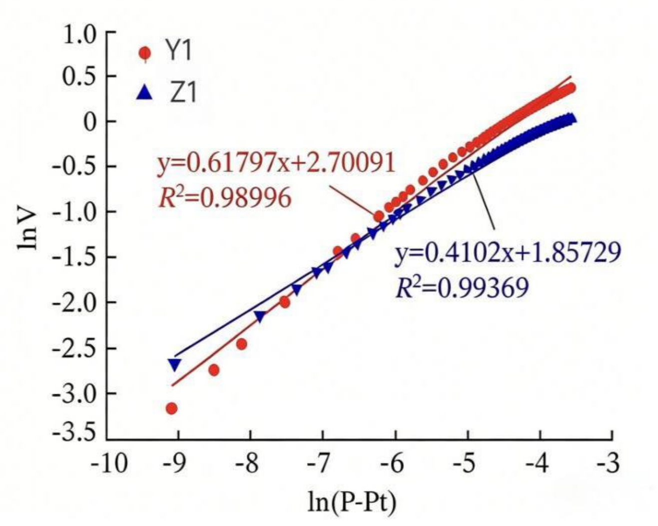

Figure 1. Schematic diagram of the Sierpinski model

Parameter definition:Generally, the fractal dimension D is not obtained by segmentation or at discrete points; instead, it is directly calculated as a single value from the relevant formula. Different models require different analytical procedures.

Advantages and limitations: The main advantage of this method lies in the small kinetic diameter of CO_2 molecules and their rapid diffusion capability at 273 K, which enables high-precision characterization of micropores (<2 nm) in coal. However, the limitation is that the measurement range is restricted to micropores or ultra-micropores only, necessitating combination with other methods to cover the full pore size range. Furthermore, the method is sensitive to test temperature and pretreatment conditions; temperature variations may affect pore structure parameters.

2.1.2. Low-Temperature Nitrogen Adsorption Method

Basic principle: The low-temperature nitrogen adsorption method is based on the theory of multilayer gas adsorption on solid surfaces (BET theory). At liquid nitrogen temperature (77 K), the nitrogen adsorption capacity of coal samples is measured under varying relative pressures, and the specific surface area, pore volume, and pore size distribution of the coal are analyzed according to the adsorption–desorption isotherms. This method exhibits high measurement accuracy for mesopores (2-50 nm), but it has limitations in characterizing micropores (<2 nm) and macropores (>50 nm). Therefore, it is usually combined with CO_2 adsorption and mercury intrusion porosimetry (MIP) methods to achieve a joint characterization of the pore structure across the full pore size range of coal reservoirs.

Fractal model: The FHH model has two common forms of calculation equations[4]:

$$\ln V = A\ln[\ln(\frac{P_0}{P})] + C$$

$$\ln\frac{V}{V_0} = A\ln[\ln(\frac{P_0}{P})] + C$$

where:P is the adsorption equilibrium pressure (MPa);P0is the saturation vapor pressure of the adsorbed gas (MPa); V is the volume of gas adsorbed at equilibrium pressure (cm^3/g); A is the slope of the double logarithmic plot of lnV versus $\ln(\ln(P_0/P))$. The fractal dimension D is linearly related to A by D=A+3.

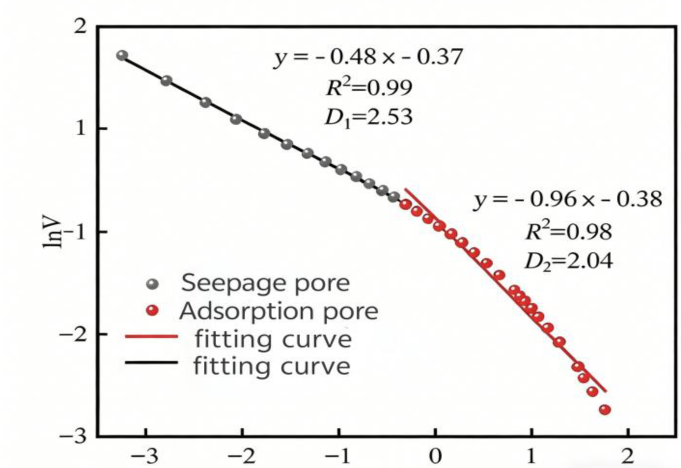

Figure 2. Schematic diagram of the FHH model

Parameter definition:Most researchers take the relative pressure P/P_0=0.45 or 0.50 as the dividing point. The region below this value is designated as the low-pressure range, and the region above as the high-pressure range; the corresponding fractal dimensions are denoted as D_1 and D_2, respectively. Here, D_1reflects the roughness of the pore surface, while D_2 reflects the complexity and developmental characteristics of the pore volume and pore structure.

Advantages and limitations: The advantage of the low-temperature nitrogen adsorption method lies in its ability to accurately characterize the specific surface area, pore volume, and pore size distribution of mesopores (2-50 nm), and the test process is non-destructive. Its limitations include the limited detection capability for micropores (<2 nm) and macropores (>50 nm), theoretical deviations of the BJH model for complex pore geometries, sensitivity to sample pretreatment conditions, and an inability to detect closed pores.

2.1.3. Mercury Intrusion Porosimetry (MIP) Method

Basic principle:The MIP method is based on the non-wetting property of mercury on coal surfaces (contact angle > 90°). According to the Washburn equation Pc=2δcosθ/r, the applied pressure P is inversely proportional to the pore throat radius r. By recording the volume of mercury intruded under different pressures, the pore size distribution is obtained. This method is more suitable for the determination of macropores; it is generally considered that the test results for pore sizes greater than 50 nm are relatively reliable. However, for micropores smaller than 2 nm, the deviation is large, and thus MIP should not be used alone.

Fractal model:The calculation equation of the Menger sponge model is as follows[5]:

$$Lg(dV/dP) = C + (\mathrm{D}-4)LgP$$

where : P is the mercury intrusion pressure (MPa);V is the volume of mercury intruded at pressure P (mL/g); and K is the slope of the double logarithmic plot of log(dV/dP) versus logP. Based on the MIP experimental data, a scatter plot of log(dV/dP)against logP is constructed, and the fractal curve and the slope K of the fitted curve are obtained. The pore fractal dimension Dpof coal is then calculated as Dp=4+K.

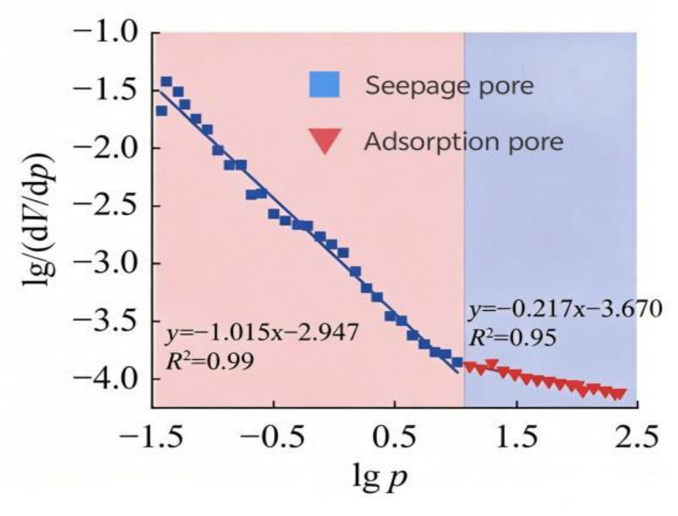

Figure 3. Schematic diagram of the Menger sponge model

Parameter definition:In most studies, a pore size threshold of 95 nm, 100 nm, or a user-defined value is adopted as the dividing point. The fractal dimension of seepage pores larger than this threshold is denoted as D_1, and that of adsorption pores smaller than this threshold as D_2. Some researchers divide the MIP fractal curve into three pressure intervals:low-pressure zone (<0.1 MPa),medium-pressure zone (0.1-10.0 MPa),and high-pressure zone (>10 MPa), with the corresponding fractal dimensions recorded as D_1, D_2, and D_3, respectively [6–7].

Advantages and limitations:The advantages of the MIP method include its simple model, rapid testing speed, and wide pore size measurement range (approximately 6 nm to 400 μm, with more accurate results for pores >50 nm), enabling the acquisition of relatively complete pore size distribution information. The limitations are that under high pressure, mercury intrusion may damage the original pore structure of coal (especially when pressures exceed 10 MPa, a compressibility correction for the pressure segment is required). This effect is particularly significant for low-rank coal and tectonically deformed coal, leading to considerable errors in the test results. Therefore, the MIP method is more suitable for medium to high-rank coals.

2.2. Multifractal

Basic principle:In multifractal analysis, the pressure or relative pressure range of mercury intrusion porosimetry (MIP), N_2 adsorption, and CO_2 adsorption experiments is taken as the total interval. This interval is divided into several sub-intervals of size ε using the bisection method. A power-law relationship between the mass probability function pi(ε) and the singularity exponent αiis defined for each subinterval[8–9]. On this basis, the partition function is calculated, from which the mass exponent and the generalized dimension spectrum are derived. Through specific equations, the multifractal singularity spectrum is constructed, thereby enabling quantitative characterization of the heterogeneity and pore connectivity of multiscale pore structures in coal reservoirs.

The power-law relationship between the mass probability function pi(ε) and the singularity exponent αi is as follows:

$$p_i(\varepsilon) \sim \varepsilon^{a_i}$$

Where: α iis the singularity exponent, which reflects the local singularity strength. A higher value of αiindicates greater smoothness, regularity, or uniformity of the data; conversely, a lower value indicates greater variability or stronger heterogeneity[10].

For boxes exhibiting multifractal behavior, the number of boxes N(ε) increases exponentially with increasing scale ε:

$$N_a(\varepsilon) \sim \varepsilon^{-f(a)}$$

where:Nα(ε) is the number of boxes whose singularity exponent lies between α and α+dα; and f(α) represents the multifractal singularity spectrum, which is the fractal dimension of the subset characterized by the same singularity exponent α. The values of α and f(α) can be calculated using the equations proposed by Chhabra and Jensen[11]:

$$a \propto \left[\sum_{i=1}^{N(\varepsilon)} \mu_i(q,\varepsilon) \ln p_i(\varepsilon) \right] / \ln \varepsilon$$

$$f(a) \propto \left[\sum_{i=1}^{N(\varepsilon)} \mu_i(q,\varepsilon) \ln \mu_i(q,\varepsilon) \right] / \ln \varepsilon$$

Where: μi(q,ε) is the family of probability measures:

$$\mu_i(q,\varepsilon) = \frac{p_i^q(\varepsilon)}{\sum_{i=1}^{N(\varepsilon)} p_i^q(\varepsilon)}$$

The partition function χ(q,ε) is defined as:

$$\chi(q,\varepsilon) = \sum_{i=1}^{N(\varepsilon)} p_i^q(\varepsilon)$$

Where:q is the statistical moment order, ranging from −∞ to +∞ (in this paper,q is taken in the range [−10,10]). When q≫1, the information from high-probability regions (dense or high-value regions) is amplified; when q≪−1, the information from low-probability regions (sparse or low-value regions) is amplified[12].
For a given q, χ(q,ε) and ε satisfy a power-law relationship:

$$\chi(q,\varepsilon) \propto \varepsilon^{-\tau(q)}$$

Where:τ(q) is the mass exponent, a characteristic function of the fractal behavior, obtained from the slope of the double-logarithmic plot of χ(q,ε) versus ε.
The generalized dimension spectrum Dqand the singularity spectrum f(α)−α are mathematically equivalent descriptions. The relationship between Dqand τ(q) is[13]:

$$\tau(q) = (q-1)D_q$$

Where:q≠1.For q<0, the behavior of low-porosity regions is emphasized; for q>0, the behavior of high-porosity regions is emphasized.
To ensure continuity of the singularity spectrum and the generalized dimension spectrum, the generalized dimension at q=1 is obtained using L'Hôpital's rule:

$$D_1 = \lim_{\varepsilon \to 0} \frac{1}{\lg \varepsilon} \sum_{i=1}^{N(\varepsilon)} p_i(1,\varepsilon) \lg[p_i(1,\varepsilon)]$$

From the obtained mass probability, partition function, mass exponent, and generalized dimension, the generalized dimension spectrum Dq−q and the multifractal singularity spectrum f(α)−α can be plotted, and the relevant multifractal parameters can be extracted. Among them,D0, D1, and D2 are the capacity dimension, information dimension, and correlation dimension, respectively.D2can be expressed using the Hurst exponent (H):

$$D_2 = 2H - 1$$

H, also known as the long-range correlation exponent, ranges from 0.5 to 1.0 and is used to describe the degree of correlation of local porosity distributions across different pore size intervals[14].

Among the multifractal parameters,H and α0 are used for the quantitative characterization of pore structure heterogeneity and pore connectivity. α0indicates the degree of concentration of pore volume distribution:a larger value of α0 implies stronger spatial variability of pore space, greater local fluctuation of pore volume, a narrower distribution interval, a greater degree of pore size distribution heterogeneity, and thus a more complex pore structure. A larger H value indicates stronger correlation of pore clusters across different pore size intervals, higher uniformity, and better pore connectivity[15].

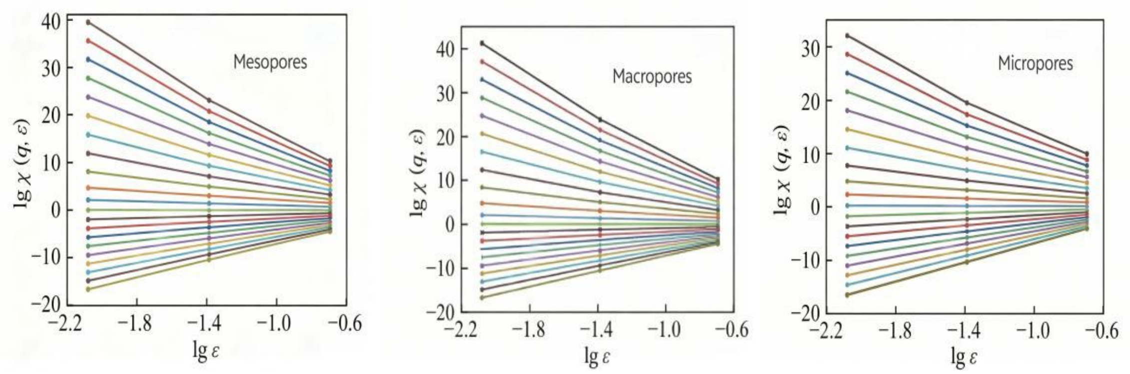

Figure 4. Partition function curves for macropores, mesopores, and micropores of coal samples

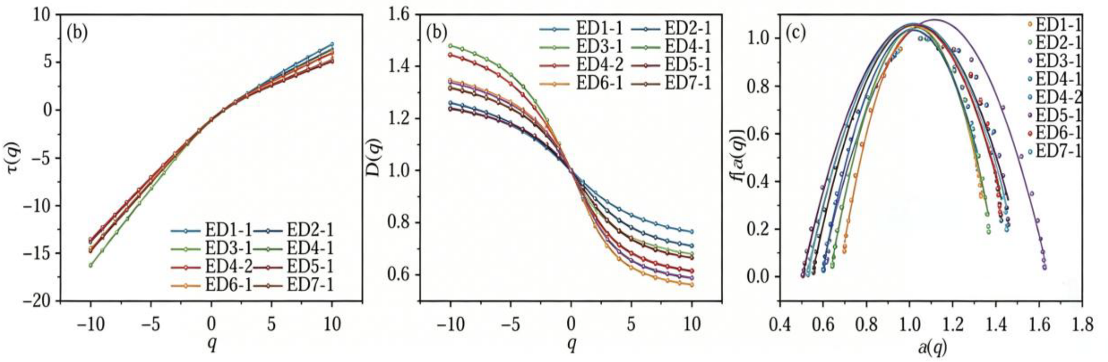

Figure 5. Multifractal characteristics of coal pore structure based on CO_2/N_2/MIP data: a. Relationship curve between the mass exponent function and the statistical moment order; b. Multifractal generalized dimension spectrum curve; c. Multifractal singularity spectrum curve

Advantages and limitations:The multifractal method can finely characterize the local heterogeneity and multi-scale distribution features of coal pores, yielding multiple parameters such as the spectral width Δα and the Hurst exponent, and is thus suitable for analyzing strongly heterogeneous coal samples. However, its computation is complex, the physical meanings of its parameters are relatively abstract, it demands high-quality data, and there is a lack of standardized operating procedures across different studies, which may introduce subjective errors.

3. Comparative Analysis of Two Fractal Methods

3.1. Theoretical Comparison

Although both monofractal and multifractal approaches fall within the realm of fractal theory, their underlying assumptions differ fundamentally.

Monofractal theory assumes that the object under study possesses uniform self-similarity across the entire scale range-i.e., the complexity of its fractal structure remains constant regardless of whether the scale is macroscopic or microscopic. Mathematically, this assumption is expressed as a power-law relationship between the target property (e.g., pore count or cumulative pore volume) and the observation scale in a double-logarithmic coordinate system, which yields a single linear trend after logarithmic transformation. The absolute value of the slope of this linear trend is the fractal dimension D. For the three-dimensional pore structure of coal, the theoretical range of the monofractal dimension is $2 \leq D \leq 3$. The closer the D value closer to 3 indicates a more complex and irregular pore structure with stronger space-filling capacity. Because the output is only a single numerical value, the monofractal dimension facilitates rapid ranking and quantitative comparison among different samples, making it particularly suitable for preliminary screening of large sample sets.

In contrast, the multifractal approach abandons the assumption of uniform fractality. It holds that complex natural systems (such as the pore network of coal) typically exhibit differentiated fractal characteristics at different spatial positions and scale intervals-i.e., local singularity coexists with global self-similarity. The multifractal method introduces a probability distribution function to quantitatively describe the degree of non-uniform aggregation of a target property (e.g., pore size distribution probability) in space. It then decomposes the entire fractal structure into multiple subsets each characterized by a distinct singularity exponent α, and separately computes the fractal dimension $f(\alpha)$ of each subset, thereby constructing a complete multifractal singularity spectrum. When this spectrum degenerates into a single peak (i.e., the spectral width $\Delta\alpha \to 0$), the multifractal reduces to a monofractal. This implies that monofractal is essentially a special case of multifractal under conditions where local variations are negligible.

In summary, from the perspective of theoretical inclusiveness, the multifractal constitutes a generalized extension of the monofractal. It not only retains the global average information that the monofractal can provide (such as the information dimension at $q=0$ in the generalized dimension spectrum), but also reveals the statistical characteristics of subsets with different singularity exponents, thereby achieving multi-level, finely detailed descriptions of pore structure heterogeneity. This theoretical advantage makes the multifractal approach irreplaceable in handling strongly heterogeneous geological materials (e.g., tectonically deformed coal and low-rank coal).

3.2. Comprehensive Comparison

To illustrate the differences between the two methods more intuitively, a multi-dimensional comparison is presented in tabular form, as shown in Table 1.

Table 1. Comprehensive comparison summary of parameters for monofractal and multifractal methods

Comparison Dimension	Monofractal	Multifractal
Output parameters	Single numerical value	Multiple parameters: $D(q)$ curve, $f(\alpha)$ spectrum, $\Delta\alpha$, H, A, etc.
Dimension of structural information	Single dimension (overall complexity)	Multi-dimension (global + local + multi-scale + connectivity)
Computational complexity	Low (linear fitting)	High (probability measure calculation, interval division, nonlinear fitting)
Data requirement	Low; insensitive to sparse data points	High; requires high-density, high signal-to-noise ratio data
Intuitiveness of results	Direct (judged by numerical value)	More complex (requires interpretation of spectral shape, width, peak, etc.)
Clarity of physical meaning	Clear (indicator of complexity)	More complex (requires geological context for interpretation)
Sample sensitivity	Insensitive (calculable with few samples)	Sensitive (requires sufficient samples for statistical stability)
Advantages	Simple and efficient, suitable for preliminary screening of large sample sets	Finely characterizes heterogeneity, reveals multi-level pore structure features
Disadvantages	Lacks ability to distinguish fractal features across pore size segments	Computationally cumbersome, parameter redundancy, sensitive to outliers
Application scenarios	Rapid evaluation, global ranking, preliminary judgment of fractal existence	Tectonically deformed coal mechanism, pore size segment study, detailed modeling, anomaly identification

From the comprehensive comparison above, it is evident that monofractal and multifractal approaches differ markedly in terms of parameter richness, computational complexity, and the ability to characterize heterogeneity. Each method has its own strengths and limitations, and neither is intrinsically superior. The key lies in selecting the appropriate method based on the research objectives, sample characteristics, and data conditions. On this basis, the following sections will further discuss the limitations of current research and future directions for development.

4. Fractal theory overview and its application in coal pore characterization

The pore hosts in coal are diverse, exhibiting multi-morphological and multi-scale characteristics and typically strong heterogeneity[16–18].Traditional Euclidean geometry has limitations in quantitatively characterizing pore heterogeneity. The fractal geometry theory proposed by Mandelbrot has been widely applied to the characterization of coal pore heterogeneity[19],including monofractal and multifractal analyses[20–21].In monofractal analysis, the fractal dimension is used to quantitatively describe pore complexity; however, this approach provides only a generalized and averaged characterization of complex structures, failing to capture their detailed features. Multifractal analysis employs continuous functions to describe self-similarity, such as the multifractal singularity spectrum and the generalized dimension spectrum, thereby providing comprehensive insight into the variation of fractal dimensions across different regions within the pore system[22–23].Multifractal can be understood as a composite system composed of multiple monofractals each with different fractal dimensions[24];its structural characteristics reflect the complexity and intrinsic singularity of the system. Multifractal analysis can also characterize the multi-scale and multi-dimensional pore size distribution features of coal, offering a new research perspective for reservoir evaluation.

Currently, both monofractal and multifractal methods have achieved substantial research results in the characterization of coal pore structures. However, significant differences exist between the two methods in terms of theoretical basis, parameter output, computational complexity, and applicable scenarios. Most existing studies have focused on the application of only one of the two methods, and systematic comparison and correlation analysis between them remain insufficient[25–27].Therefore, clarifying the differences and applicable scopes of the two methods is of great significance for promoting the standardized application of fractal theory in coal pore research.

5. Current Limitations and Future Perspectives

Major limitations of current research:

1) Predominance of single characterization and lack of synergistic application:Most current studies employ either monofractal or multifractal methods in isolation, rarely combining the two approaches systematically. This precludes the simultaneous satisfaction of both global evaluation and local detailed characterization requirements.
2) Widespread misconception of direct cross-model comparison:Different fractal models (e.g., FHH model, Menger model, Sierpinski model) differ in their theoretical assumptions, applicable pore size ranges, and calculation formulas. Directly comparing the D values obtained from different models lacks theoretical justification, yet such practices remain common in the literature.
3) Strong subjectivity in fractal model selection and lack of adaptability assessment criteria:Multiple fractal models correspond to different experimental data. Researchers often select models subjectively based on experience, and the same dataset may yield significantly different results when different models are applied. There is currently no unified criterion for model adaptability assessment.
4) Insufficient interpretation of the geological significance of multifractal parameters:Although multifractal analysis can output parameters such as $\Delta\alpha$ and H, the quantitative relationships between these parameters and geological controlling factors-such as coal rank, maceral composition, and tectonic deformation-still need to be further clarified.
5) Lack of objective criteria for selecting fractal scaling intervals:The

determination of linear scaling intervals often relies on subjective observation, lacking quantitative and repeatable methods, which affects the consistency and comparability of the results.

Future perspectives:

1) Establish a "monofractal-first, multifractal-second" hierarchical characterization workflow:It is recommended to use monofractal analysis as a rapid screening tool to identify typical samples, followed by in-depth multifractal analysis, thereby forming a standardized work procedure.
2) Develop cross-model normalization comparison methods:Through strategies such as calibration using reference samples and uniform truncation of linear intervals, establish a comparability framework for the results obtained from different fractal models.
3) Construct a machine-learning-based fractal model adaptation system:Train models using published data to automatically recommend the most suitable fractal model and parameters according to coal rank and pore size distribution characteristics.
4) Deepen the geological application of multifractal parameters:Establish quantitative relationships between $\Delta\alpha$, H and practical indices such as tectonically deformed coal types, gas outburst hazard, and coalbed methane recoverability, thereby promoting engineering applications.
5) Strengthen quantitative correlation studies between fractal dimension and geological controlling factors:Systematically establish empirical equations linking fractal dimension with intrinsic factors including coal rank, maceral composition, and ash content, so as to enhance the predictive capability of fractal parameters in reservoir evaluation.

6. Conclusions

(1) Monofractal analysis, through the combination of models based on CO2 adsorption, N2 adsorption, and mercury intrusion porosimetry (MIP) data, can directly achieve continuous quantitative characterization of fractal features across the full pore size range of coal reservoirs. In contrast, multifractal analysis requires the integration of the three types of data into a continuous full-pore-size interval. Based on the partition function and the scale power-law relationship, the mass exponent $\tau(q)$ is obtained, from which the generalized dimension spectrum Dq and the singularity spectrum $f(\alpha)-\alpha$ are derived, enabling a unified characterization of local heterogeneity and multi-scale features.

(2) Fractal theory (including both monofractal and multifractal approaches) provides an effective tool for the quantitative characterization of coal pore heterogeneity. However, the two methods differ fundamentally in theoretical basis and information-describing capability. Current studies have mostly focused on only

one of the two approaches, and systematic comparison and correlation analysis between them remain insufficient. Therefore, clarifying the differences and applicable scopes of monofractal and multifractal analyses is of significant theoretical importance for promoting the standardized application of fractal theory in coal pore research.

(3) The monofractal approach is computationally simple and suitable for global pore evaluation, whereas the multifractal approach is rich in information and well-suited for in-depth analysis of strongly heterogeneous coal samples. The two methods complement each other rather than substituting for one another.

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