

Article

Differences in Nano–Mesopore Structure and Fractal Characteristics of Coal Samples from the Xishanyao with Different Maceral Compositions

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Abstract

The pore system of coal reservoirs is the fundamental structural basis controlling coalbed methane adsorption, storage, diffusion, migration, and production performance. Its development characteristics are influenced not only by thermal maturity but also by maceral composition. To clarify the differences in mesopore structure and fractal characteristics of coal samples with different maceral compositions, this study focuses on the Xishanyao Formation coals in the Nileke Depression, northeastern Yili Basin. Ten coal samples were collected and analyzed using coal petrology and coal quality tests, low-temperature nitrogen adsorption experiments, and mono-fractal and multifractal characterization. The results show that the samples have $R_{o,max}$ values ranging from 0.70% to 1.31%, indicating broadly comparable thermal maturity, whereas vitrinite and inertinite contents vary significantly. Accordingly, the samples can be classified into vitrinite-rich Type I and relatively low-vitrinite Type II. Low-temperature nitrogen adsorption results indicate that both types contain mesopores within the 2–100 nm range, but they differ markedly in pore-size distribution and hysteresis-loop characteristics. Type I is mainly controlled by the 10–50 nm pore-size interval and is characterized by a relatively concentrated distribution of medium-scale mesopores, whereas Type II is more strongly influenced by the 50–100 nm interval and shows a more dispersed pore distribution. Fractal analysis further reveals systematic differences between the two types in pore-surface roughness, structural complexity, and scale-dependent heterogeneity. Type I is mainly characterized by enhanced pore-structure complexity governed by medium-scale mesopores, whereas Type II is more strongly characterized by enhanced heterogeneity controlled by variations in larger-scale mesopores. Overall, differences in maceral composition influence the complexity and multi-scale heterogeneity of the mesopore system by controlling the dominant pore-size intervals and pore-organization patterns. These findings provide a geological basis for reservoir evaluation of the Xishanyao Formation coals and for understanding the mechanisms of coalbed methane occurrence and migration.

Keywords: deep coalbed methane; coal macerals; mesopore structure; low-temperature nitrogen adsorption; mono-fractal; multifractal; pore heterogeneity



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1. Introduction

Coal pore systems provide the space for methane adsorption and storage and influence gas diffusion, seepage, and production behavior. In deep coal reservoirs, pore development is affected by several factors, including coal rank, maceral composition, mineral matter, tectonic modification, and burial-related diagenesis. Mesopores are particularly relevant because they contribute to both pore volume and specific surface area and may connect smaller adsorption pores with larger seepage spaces. Therefore, identifying the factors that control mesopore development is important for reservoir characterization and for understanding methane occurrence in deep coal seams [1–3]. Previous studies have shown that the pore–fracture system of coal reservoirs can generally be classified into micropores (<2 nm), mesopores (2–100 nm), and macropores (100–10,000 nm). Among them, mesopores (2–100 nm) are not only an important source of specific surface area, but also key structural units linking adsorption space with migration pathways. Therefore, characterization of mesopore development is of great significance for the refined evaluation of coal reservoirs and for improving CBM productivity.

Low-temperature liquid adsorption experiment (LT N₂ GA) has become an important technique for characterizing coal pore structures because of its high sensitivity to subtle pore-structure variations and its ability to effectively characterize pore-size distribution, pore volume, and specific surface area within the 2–100 nm range. Lu et al. (2024), based on LT N₂ GA and low-field nuclear magnetic resonance (NMR) experiments, showed that pores of different size ranges are well developed and well connected in low-rank coals, whereas the connectivity among transition pores, mesopores, and macropores is relatively poor in medium-rank coals, and numerous micropores in high-rank coals are closed or semi-closed [1]. Wang et al. (2024), using low-pressure CO₂/N₂ adsorption and fractal analysis, reported that thermal evolution leads to reduced pore volume, enlarged average pore size, and smoother pore surfaces, and that changes in micropore structure are closely related to methane adsorption capacity [2]. Zhang et al. (2025), based on low-temperature N₂ and CO₂ adsorption experiments, found that tectonic deformation can significantly reconstruct coal pore structures, as evidenced by overall increases in pore volume, specific surface area, and fractal dimension with increasing deformation intensity, while micropores contribute much more than mesopores to total pore volume and specific surface area [3].

Fractal theory has been widely used to describe the irregular geometry and heterogeneous distribution of coal pores [4–6]. Early studies distinguished the fractal responses of adsorption pores and seepage pores and discussed their relationships with methane adsorption capacity and permeability [7,8]. Subsequent studies applied geometric, thermodynamic, low-field NMR, low-temperature gas adsorption, and mercury-intrusion methods to characterize pore complexity at different scales [9–17]. Multifractal analysis provides additional information because it reflects local variations in pore distribution rather than only average pore characteristics [18,19]. Recent studies have further combined fractal analysis with low-temperature adsorption, NMR, CT imaging, and other multiscale characterization methods to evaluate pore heterogeneity in coal reservoirs [1,20–23]. The multiscale concept of fractal analysis has also been used for complex heterogeneous surfaces in other porous materials [24].

Previous studies have shown that coal rank, tectonic deformation, mineral matter, and maceral composition may all affect coal pore structure [5,6,20,25–30]. However, many published studies include samples with different coal ranks, deformation histories, or depositional backgrounds. Under such conditions, the individual effect of maceral composition is difficult to distinguish. Recent work on vitrain, durain, inertinite-rich coal, and deep coal reservoirs has shown that differences in organic composition may be accompanied by differences in pore development and methane adsorption behavior [20–23,30]. Nevertheless, the

extent to which maceral assemblages are associated with dominant mesopore intervals and fractal heterogeneity under a comparable maturity range remains insufficiently understood.

The Xishanyao Formation coal samples from the Nileke Depression provide a suitable case for this comparison because they show marked differences in vitrinite and inertinite contents while remaining within a moderate maturity range. This study therefore combines coal petrology, coal quality analysis, low-temperature nitrogen adsorption, mono-fractal analysis, and multifractal analysis to compare mesopore structure and heterogeneity between vitrinite-rich and relatively low-vitrinite coal samples. The purpose is not to establish a universal classification for all coals, but to examine the pore-structure response of these samples under the geological conditions of the study area (Figure 1).

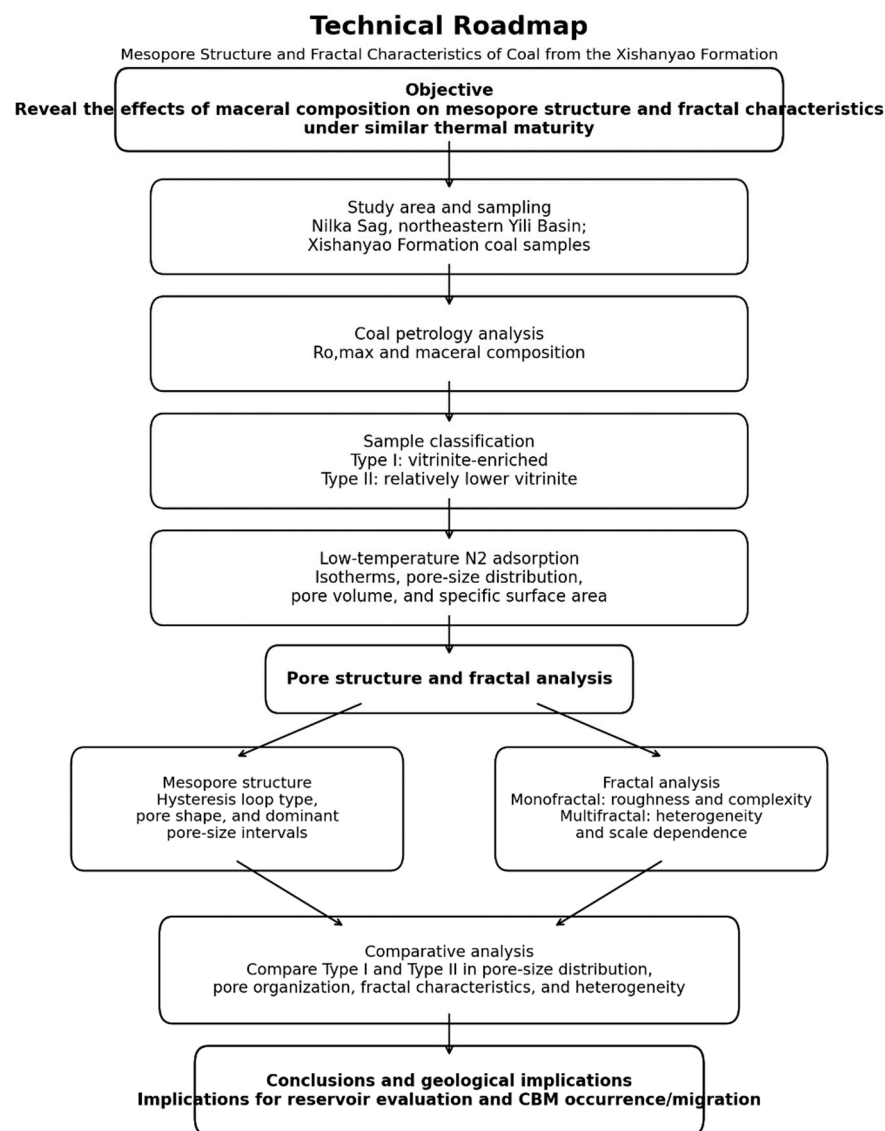


Figure 1. Technical roadmap for the study of mesopore structure and fractal characteristics of Xishanyao Formation coal samples.

2. Geological Setting and Experimental Methods

2.1. Geological Setting and Sample Collection

The study area is located in the Nileke Depression in the northeastern Yili Basin, which is a typical Meso–Cenozoic intermontane fault-depression basin. It is elongated in an approximately east–west direction, bounded by the Borohoro Mountains to the north and the Awulale Mountains to the south. From south to north, it can be divided into three

secondary structural units: the Kashi River intermontane sag, the Tamuletike fault depression, and the Awulale composite anticline. The Jurassic strata are relatively well developed in the study area and, from bottom to top, mainly comprise the Badaowan Formation, Sangonghe Formation, and Xishanyao Formation. Among them, the Xishanyao Formation is an important coal-bearing unit and the main target horizon for coalbed methane exploration in the study area. This formation was deposited in lacustrine and swamp environments and is composed of a succession of gray to yellowish-green sandstones, mudstones, siltstones, coarse sandstones, and coal seams. A set of very thick-bedded sandy conglomerates occurs at the base and serves as the marker bed separating the Xishanyao Formation from the Sangonghe Formation. Overall, it represents a typical continental coal-bearing clastic succession. Previous studies have shown that the Xishanyao Formation contains 9–15 coal seams, with seam thicknesses ranging from 0.29 to 100.23 m. The number of minable coal seams is generally 5–8, and the cumulative thickness of minable seams ranges from 22.57 to 69.88 m. The major minable seams are mainly concentrated in the lower and middle intervals of the formation, showing relatively good stratigraphic concentration and lateral continuity.

A total of 10 coal samples were selected for systematic analyses. Their $R_{o,max}$ values range from 0.70% to 1.31%, indicating broadly comparable thermal maturity at a moderate evolutionary stage. In contrast, maceral composition varies considerably among the samples, with vitrinite contents of 21.89–91.04%, inertinite contents of 1.08–75.09%, and generally low liptinite contents that increase only in a few samples. These results indicate that the most significant differences among the samples are related not to coalification stage, but to maceral assemblages.

2.2. Experimental Methods and Theory

(1) Coal petrology and coal quality analyses

The maximum vitrinite reflectance ($R_{o,max}$) and maceral composition were determined using an optical microscope 23-750VI (Ningbo Sunny Instruments Co., Ltd., Ningbo, China) coupled with a microspectrophotometer, following the Chinese national standard GB/T 6948-2008 [31].

(2) Pore characterization

Low-temperature nitrogen adsorption experiments were performed using an ASAP 2460 automatic gas adsorption analyzer (Micromeritics Instrument Corp., Norcross, GA, USA) according to the Chinese national standard GB/T 19587-2017 [32]. The experiments were mainly used to characterize mesopore properties in the 2–100 nm range.

(3) Mono-fractal and multifractal analyses

To quantitatively characterize the complexity of the coal pore system, mono-fractal and multifractal theories were applied. Mono-fractal analysis was used to describe pore-surface roughness and structural complexity, whereas multifractal analysis was employed to identify pore-distribution differences across local regions and scales, thereby characterizing the heterogeneity and scale-dependent variability of the pore system. In this study, the FHH method was applied to estimate fractal dimensions within the 2–100 nm pore-size range. The FHH model combines adsorption data with a power-law relationship and is capable of describing the irregularity of pore surfaces and spatial structures.

$$\ln\left(\frac{V}{V_m}\right) = C + A \left[\ln\left(\ln\left(\frac{P_0}{P}\right)\right) \right] \quad (1)$$

where P is the equilibrium pressure (MPa), P_0 is the saturation vapor pressure (MPa), V is the adsorbed volume at equilibrium pressure ($\text{cm}^3 \cdot \text{g}^{-1}$), V_m is the monolayer adsorption

capacity ($\text{cm}^3 \cdot \text{g}^{-1}$), C is a fitting constant, and A is the power-law exponent related to the adsorption mechanism and fractal dimension.

Previous studies have shown that the relationship between A and fractal dimension varies with adsorption state. Based on the characteristics of the coal adsorption data, $D_N = A + 3$ was adopted in this study to characterize the geometric complexity of the mesopore structure more reasonably.

3. Results

3.1. Sample Classification

According to Table 1 and Figure 2, the $R_{o,max}$ values of the samples range from 0.70% to 1.31%, placing all samples within a moderate maturity range. The samples nevertheless show clear differences in maceral composition, particularly in vitrinite and inertinite contents. For descriptive comparison, the samples were divided into two groups according to vitrinite content: Type I includes vitrinite-rich samples with vitrinite content $\geq 60\%$, whereas Type II includes samples with vitrinite content $< 60\%$ and relatively higher inertinite content. Figure 2a shows that the two groups partly overlap in $R_{o,max}$, whereas Figure 2b shows a clear contrast in vitrinite content. Therefore, the subsequent comparison focuses on the relationship between maceral assemblages and pore characteristics within this sample set. This grouping does not completely remove the possible influence of maturity, but it helps reduce the effect of large compositional differences when comparing the two sample types.

Table 1. Sample list and petrographic parameters.

Sample	$R_{o,max}$ %	Vitrinite %	Liptinite %	Inertinite %	Mineral Matter %
S1	1.31	89.14	0	8.99	1.87
S2	1.23	87.01	0	11.42	1.57
S3	1.19	33.61	1.66	56.43	8.3
S4	1.19	58.65	0	25.56	15.79
S5	1.21	21.89	0.38	75.09	2.64
S6	1.17	91.04	0	1.08	7.88
S7	1.08	70.86	0	26.98	2.16
S8	1.11	76.95	0	9.66	13.39
S9	0.7	33	6.27	59.08	1.65
S10	0.71	51.58	6.66	41.06	0.7

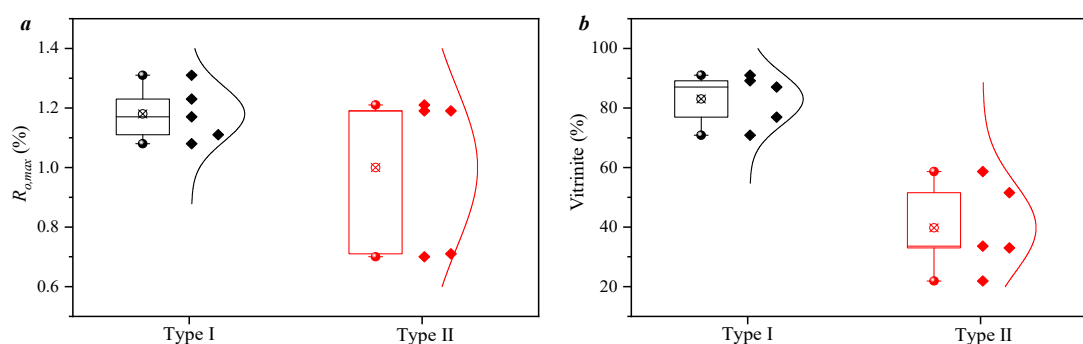


Figure 2. Distribution of $R_{o,max}$ (a) and vitrinite content (b) in Type I and Type II coal samples. Type I includes S1, S2, S6, S7, and S8, with vitrinite content $\geq 60\%$; Type II includes S3, S4, S5, S9, and S10, with vitrinite content $< 60\%$.

3.2. Nanopore Structure

Figure 3 shows that all coal samples display typical mesopore adsorption characteristics in their nitrogen adsorption–desorption isotherms, although the hysteresis-loop morphology differs markedly between the two sample types. Type I samples are characterized by a steep adsorption branch near saturation pressure and a sharp desorption branch at intermediate relative pressures, producing a relatively wide hysteresis loop. A distinct inflection point in the desorption branch occurs at around $P/P_0 \approx 0.5$, indicating that the pore system likely contains slit-shaped pores, cylindrical pores, and related combined pore types (Figure 3a). In contrast, Type II samples exhibit a very steep adsorption branch near saturation pressure, whereas the desorption branch remains generally close to the adsorption branch, resulting in a relatively narrow hysteresis loop. This suggests that the pore system may contain wedge-shaped semi-closed pores, slit-shaped pores, and ink-bottle pores (Figure 3b).

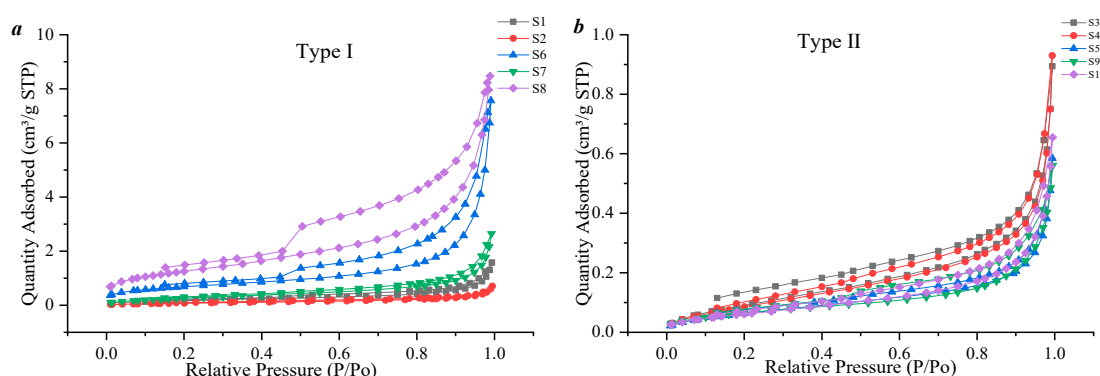


Figure 3. Low-temperature N_2 adsorption–desorption isotherms of Type I (a) and Type II (b) coal samples. Type I includes vitrinite-rich samples S1, S2, S6, S7, and S8; Type II includes relatively low-vitrinite samples S3, S4, S5, S9, and S10.

In Type I samples, the incremental pore volume of S6 and S8 displays a unimodal distribution, with peaks at 90–100 nm, whereas the other samples show a gradual increase with increasing pore size (Figure 4a). This pattern suggests that, although vitrinite enrichment provides a broadly similar organic framework, differences in coal-forming material composition, compaction, and local mineral infilling still lead to different mesopore development modes. Consequently, some samples are dominated by concentrated development in the larger pore-size interval, whereas others exhibit a progressive increase in pore volume toward larger pore sizes. In contrast, all Type II samples show an increasing trend in incremental pore volume, but the increase is much weaker than that in Type I (Figure 4b), indicating that a distinct dominant pore-size interval is less well developed. This is likely related to the relatively lower vitrinite contents and higher inertinite contents of Type II, which weaken continuous pore formation and subsequent modification within the organic framework.

Likewise, in Type I, the incremental specific surface area of S6 and S8 shows a bimodal distribution, with peaks at 2–5 nm and around 30 nm, whereas the other samples exhibit a unimodal peak at 2–5 nm. This indicates that small mesopores are the principal contributors to specific surface area, while medium-scale mesopores are also relatively well developed in some samples. In Type II, all samples display a unimodal distribution with a peak at 2–5 nm, but the peak values are generally lower than those of Type I (Figure 5). This suggests that small mesopores are less abundant and less developed in Type II, resulting in a lower overall specific surface area.

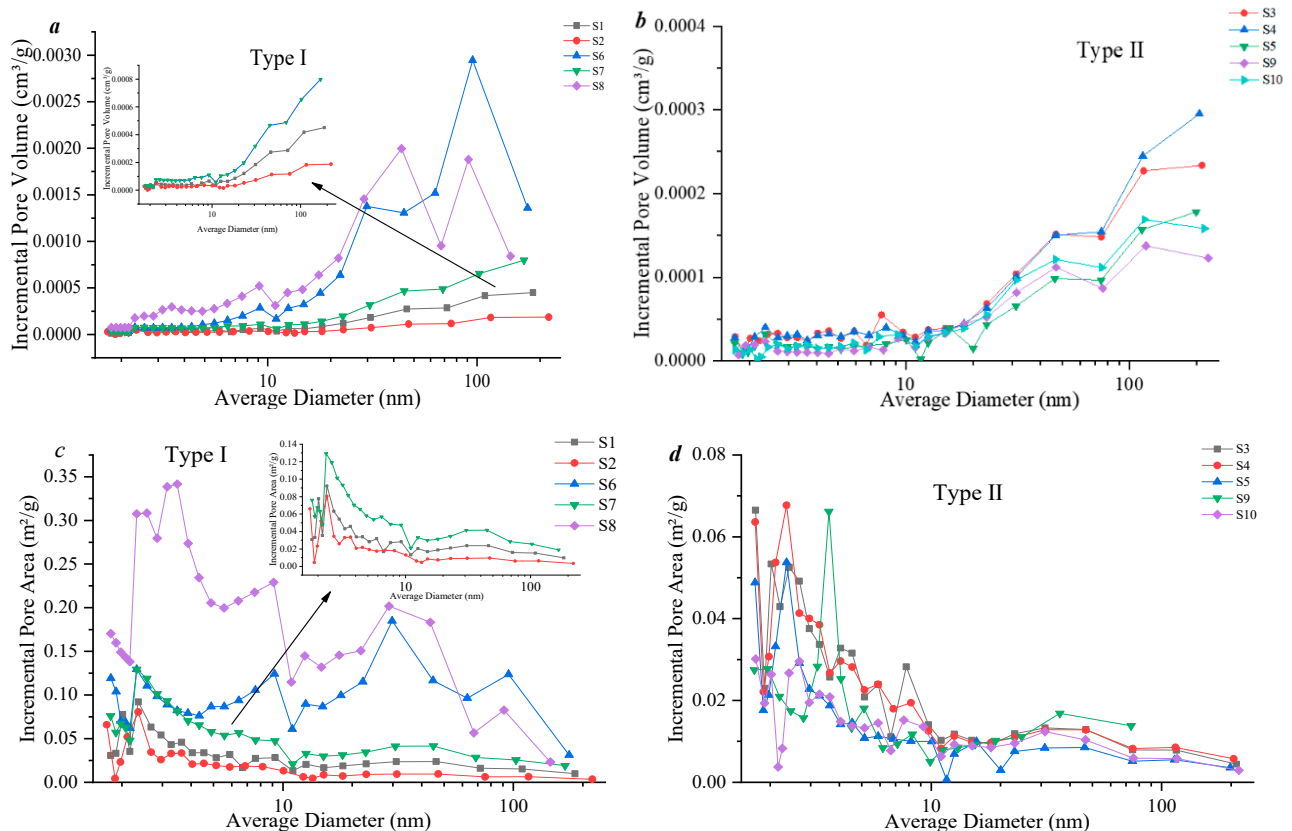


Figure 4. Incremental pore-volume and incremental specific-surface-area distributions of Type I and Type II coal samples: (a) pore-volume distribution of Type I; (b) pore-volume distribution of Type II; (c) specific-surface-area distribution of Type I; and (d) specific-surface-area distribution of Type II. Sample codes are defined in Table 1.

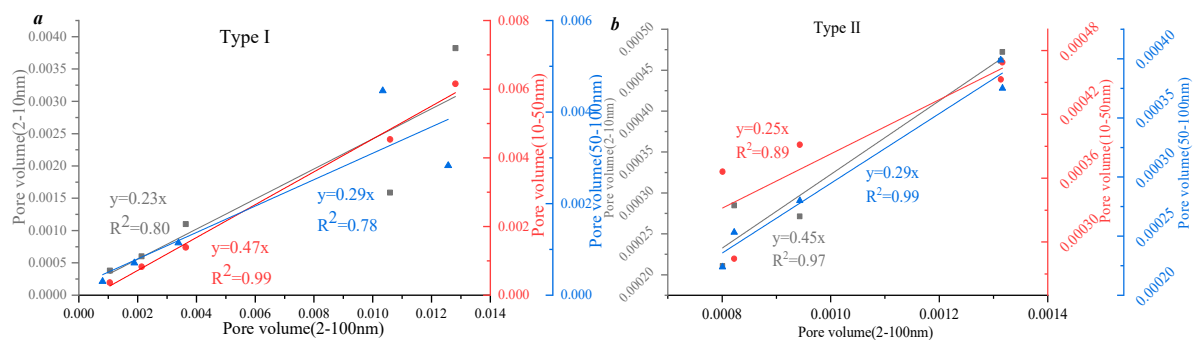


Figure 5. Fitting relationships between pore volume in different pore-size intervals and total mesopore volume in Type I and Type II coal samples ((a), fitting relationships between pore volume in different pore-size intervals and total mesopore volume in Type I coal samples; (b), fitting relationships between pore volume in different pore-size intervals and total mesopore volume in Type II coal samples).

In Type I samples, the total mesopore volume shows the strongest correlation with pore volume in the 10–50 nm interval, whereas its correlations with the 2–10 nm and 50–100 nm intervals are relatively weaker, indicating that medium-scale mesopores in the 10–50 nm range are the key interval controlling variations in total mesopore volume. This is because, although 2–10 nm small mesopores contribute substantially to specific surface area, their pore volume is limited; by contrast, pores in the 50–100 nm interval are developed only in some samples and show relatively poor continuity and stability. In comparison, the 10–50 nm interval provides a better balance between pore abundance and single-pore

volume contribution, and therefore more directly reflects the overall development of mesopores in Type I samples (Figure 5a).

In Type II samples, the total mesopore volume shows the strongest correlation with pore volume in the 50–100 nm interval, whereas its correlations with the 2–10 nm and 10–50 nm intervals are relatively lower, indicating that larger-scale mesopores exert a more significant control on variations in total pore volume. This is because Type II samples have relatively lower vitrinite contents and higher inertinite contents, and the overall mesopore development is weaker; moreover, small- and medium-scale pores are more dispersed and fail to form a stable dominant pore-size interval. Once the 50–100 nm interval becomes more developed, it makes a more pronounced incremental contribution to total pore volume. Overall, Type I is mainly characterized by a pore structure dominated by medium-scale mesopores, whereas Type II is characterized by a pore structure controlled by larger-scale mesopores (Figure 5b).

Mineral matter shows relatively higher positive correlations with pore volume and specific surface area than vitrinite and inertinite. This pattern suggests that mineral-associated pores and pore–mineral interfaces may contribute to mesopore development in some Type I samples. Within the pore-size comparison, the 10–50 nm interval shows correlation patterns that are most similar to those of total mesopore volume. This suggests that medium-scale mesopores are an important contributor to variation in total mesopore volume in Type I samples (Figure 6a).

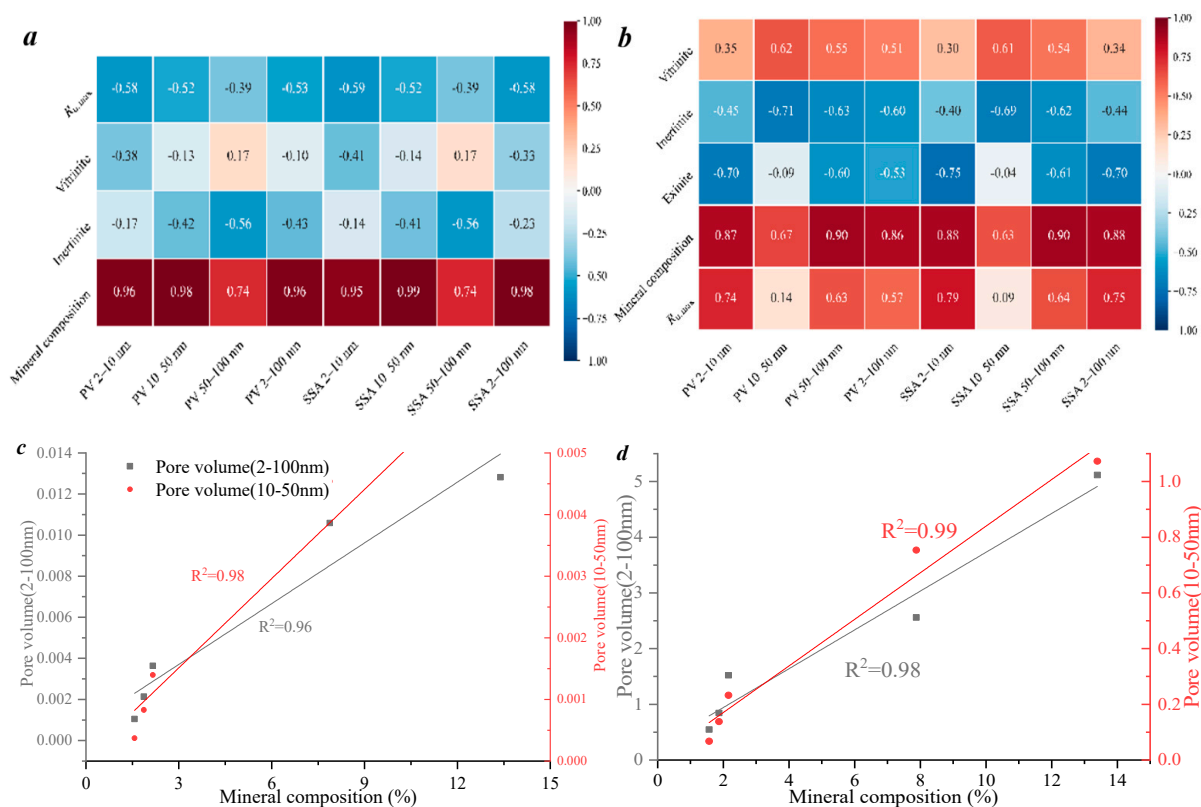


Figure 6. Correlation patterns between maceral composition, $R_{o,max}$, and mesopore parameters in Type I and Type II coal samples: (a) correlation heat map for Type I; (b) correlation heat map for Type II; (c) selected relationships between mineral matter and pore-volume variables in Type I; and (d) corresponding relationships in Type II. The pore-size intervals shown in panels (c,d) are identified directly on the axes.

Mineral matter is positively correlated with several pore-structure parameters, whereas inertinite tends to show negative correlations. $R_{o,max}$ also shows moderate correlations

with some pore parameters. These results suggest that mesopore development in Type II samples may reflect the combined effects of maceral composition, mineral matter, and maturity-related evolution rather than the influence of a single factor. For Type II, the 50–100 nm interval shows correlation patterns most similar to those of total mesopore volume. This suggests that larger mesopores make a relatively greater contribution to the variation in total mesopore volume within this group (Figure 6b).

In Type I, the correlation between pore volume in the 10–50 nm interval and total mesopore volume is closest to that of mineral matter, whereas in Type II the closest relationship is found for the 50–100 nm interval. This indicates a clear difference in the dominant pore-size scale controlling total mesopore volume between the two sample types, namely that Type I is mainly characterized by a pore structure dominated by medium-scale mesopores, whereas Type II is characterized by a pore structure controlled by larger-scale mesopores (Figure 6c,d). This is because a vitrinite-rich background is more favorable for the formation and preservation of medium-scale mesopores, which not only contribute to pore volume but also serve as structural links, whereas the relatively higher inertinite content and weaker continuity of pore formation in Type II makes it difficult for small- and medium-scale pores to develop in a concentrated manner, so that changes in larger pores are more likely to affect the overall pore structure. These differences indicate that mesopore differentiation under different maceral-composition backgrounds is reflected not only in the magnitude of pore parameters, but also in the dominant pore-size scale corresponding to total mesopore volume.

3.3. Fractal Characteristics of Coal Pores

The mono-fractal dimension of Type I ranges from 2.513 to 2.580, with an average of 2.539, whereas that of Type II ranges from 2.499 to 2.562, with an average of 2.525 (Figure 7a,b). The fractal dimensions of both types are significantly greater than 2, indicating that the mesopore surfaces of the coal samples in the study area are characterized by strong heterogeneity (Figure 7). The average fractal dimension of Type I is slightly higher than that of Type II, suggesting that its pore surfaces are rougher. This is because Type I samples are mainly controlled by medium-scale mesopores in the 10–50 nm interval, which not only provide relatively large specific surface area but also more readily develop heterogeneous pore morphologies, thereby exhibiting stronger surface fractal characteristics. By contrast, the fractal dimension of Type II is slightly lower overall, indicating that although larger-scale mesopores make a more obvious contribution to total pore volume, pore-surface roughness and surface complexity are relatively weaker. This is because Type II samples are mainly influenced by the 50–100 nm interval, in which the increase in larger pore sizes is expressed more as pore-space expansion than as increasing pore-surface complexity.

Type I has $D_{min}-D_0$ values ranging from 0.268 to 0.766, with an average of 0.556; D_0-D_{max} values ranging from 0.879 to 0.949, with an average of 0.907; and $D_{min}-D_{max}$ values ranging from 1.147 to 1.674, with an average of 1.463. In comparison, Type II has $D_{min}-D_0$ values of 0.197–0.791, with an average of 0.384; D_0-D_{max} values of 0.885–0.912, with an average of 0.899; and $D_{min}-D_{max}$ values of 1.083–1.703, with an average of 1.283 (Figure 8). Figure 8c–e further shows that these multifractal parameters are generally higher in Type I than in Type II, indicating that the mesopore system of Type I exhibits larger multiscale fluctuations, stronger local heterogeneity in pore distribution, and more pronounced multifractal characteristics overall. This is because Type I samples are mainly controlled by medium-scale mesopores in the 10–50 nm interval, which are not only major contributors to total pore volume and specific surface area, but also the pore-size interval most sensitive to variations in pore-surface roughness and pore-throat configuration. Although Type II samples also display multifractal characteristics, their

fractal parameters are generally lower, and local heterogeneity is weaker than that of Type I. This is because Type II samples are mainly influenced by the 50–100 nm interval, where the increase in larger-scale mesopores is expressed mainly as pore-space expansion rather than stronger local pore heterogeneity.

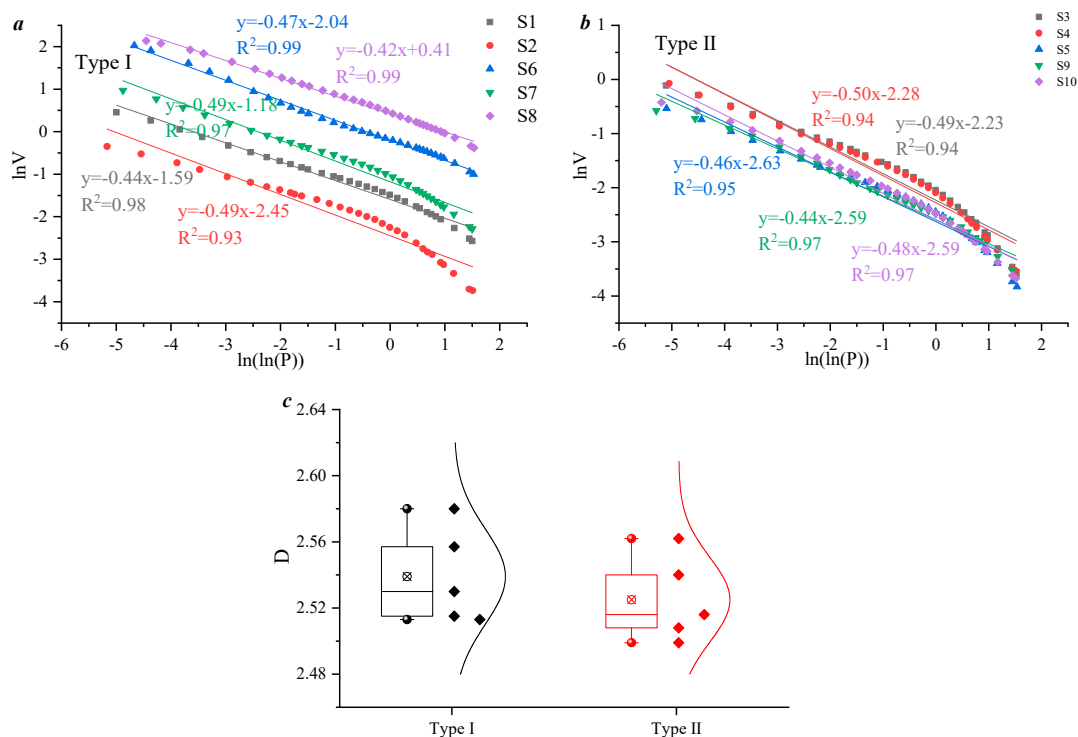


Figure 7. Mono-fractal of Type I and Type II coal samples ((a), FHH fitting curves for the mono-fractal dimension of Type I coal samples; (b), FHH fitting curves for the mono-fractal dimension of Type II coal samples; (c), distribution of mono-fractal dimensions in Type I and Type II coal samples).

In Type I, $D_{min}-D_0$ shows a significant positive correlation with $D_{min}-D_{max}$ ($R^2 = 0.99$), whereas D_0-D_{max} exhibits a nonlinear positive correlation with $D_{min}-D_{max}$. This indicates that the overall multifractal characteristics of Type I are mainly controlled by $D_{min}-D_0$, meaning that the difference between the high-value region of pore distribution and the average state is the key factor governing multifractal variation. This is because Type I samples are mainly controlled by medium-scale mesopores in the 10–50 nm interval, which not only make important contributions to total pore volume and specific surface area but are also highly sensitive to variations in pore-surface roughness and pore-throat configuration, thereby favoring local pore clustering and heterogeneity.

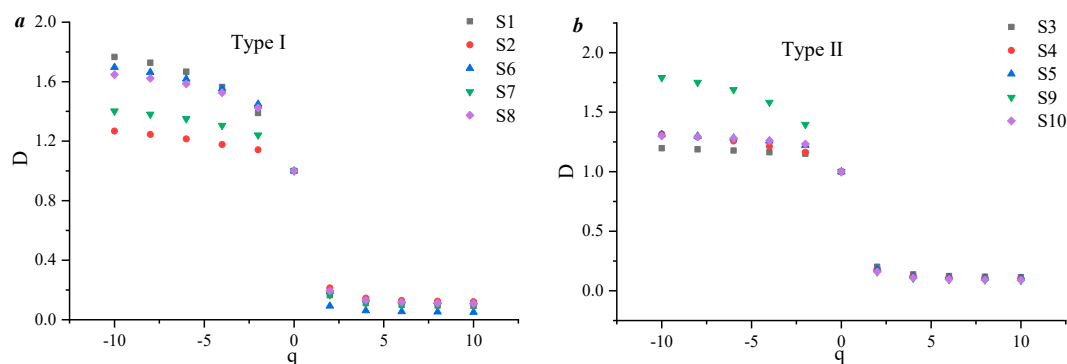


Figure 8. Cont.

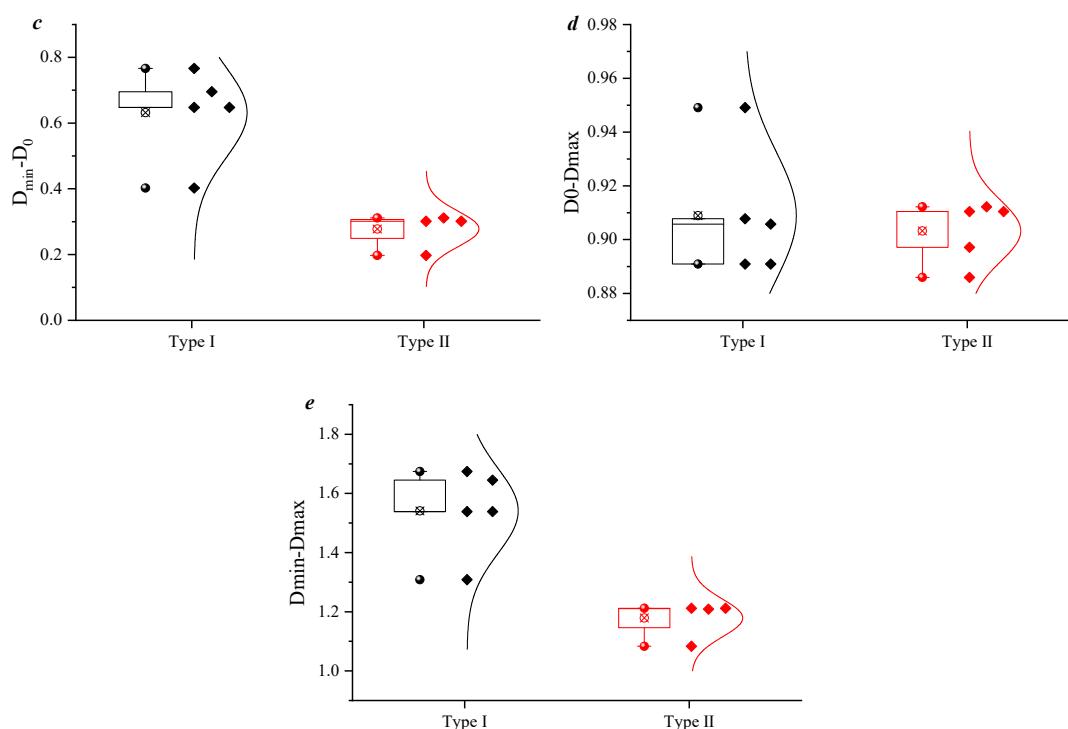


Figure 8. Multifractal spectra and parameter distributions of Type I and Type II coal samples ((a), multifractal spectra of Type I coal samples; (b), multifractal spectra of Type II coal samples; (c), distribution of $D_{min}-D_0$ in Type I and Type II coal samples; (d), distribution of D_0-D_{max} in Type I and Type II coal samples; (e), distribution of $D_{min}-D_{max}$ in Type I and Type II coal samples).

In Type II, $D_{min}-D_0$ also shows a significant positive correlation with $D_{min}-D_{max}$ ($R^2 = 0.99$), whereas D_0-D_{max} is positively correlated with $D_{min}-D_{max}$ ($R^2 = 0.70$). This suggests that the overall multifractal characteristics of Type II are likewise mainly controlled by $D_{min}-D_0$, although D_0-D_{max} also contributes to multifractal variation to some extent. This is because Type II samples are mainly controlled by larger-scale mesopores in the 50–100 nm interval, and changes in larger pore sizes not only modify the volumetric distribution of local pore-enriched zones, but also enhance the difference between low-value regions of pore distribution and the average state (Figure 9).

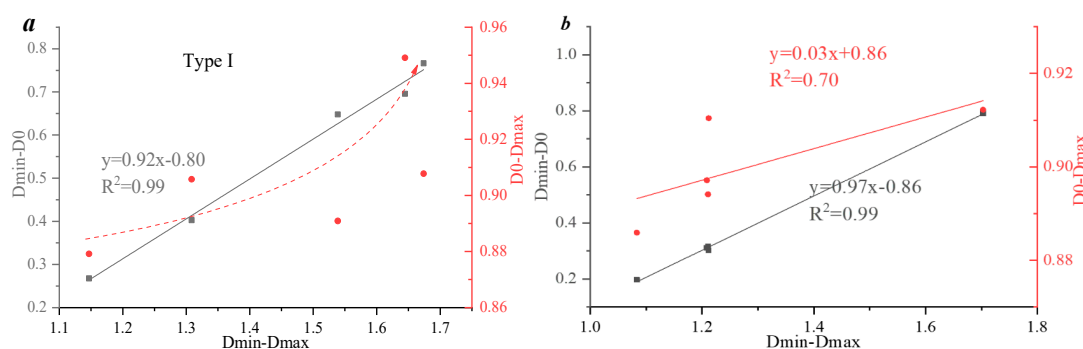


Figure 9. Fitting relationships among multifractal parameters of Type I and Type II coal samples ((a), fitting relationships of $D_{min}-D_0$ and D_0-D_{max} with $D_{min}-D_{max}$ in Type I coal samples; (b), fitting relationships of $D_{min}-D_0$ and D_0-D_{max} with $D_{min}-D_{max}$ in Type II coal samples).

Figure 10a,b show that the mono-fractal dimension D has the strongest correlation with total pore volume in both sample types, with correlation coefficients of 0.57 and -0.87 for Type I and Type II, respectively. This indicates that pore-volume variation is primarily expressed as changes in pore-surface roughness and morphological complexity. By comparison, the correlations between multifractal parameters and pore volume are relatively weaker, suggesting that local-scale heterogeneity is not the primary response to pore-volume variation. In Type I, $D_{min}-D_{max}$ ($R^2 = 0.51$) and $D_{min}-D_0$ ($R^2 = 0.50$) show relatively high correlations, indicating that pore-volume increases in this sample type mainly correspond to the enhancement of high-value regions and the expansion of overall heterogeneity. In contrast, D_0-D_{max} shows the strongest correlation in Type II ($R^2 = -0.77$), indicating that the development of larger-scale mesopores mainly enhances the difference between low-value regions and the average state, thereby reflecting a heterogeneous pore structure mainly controlled by larger pore-size intervals.

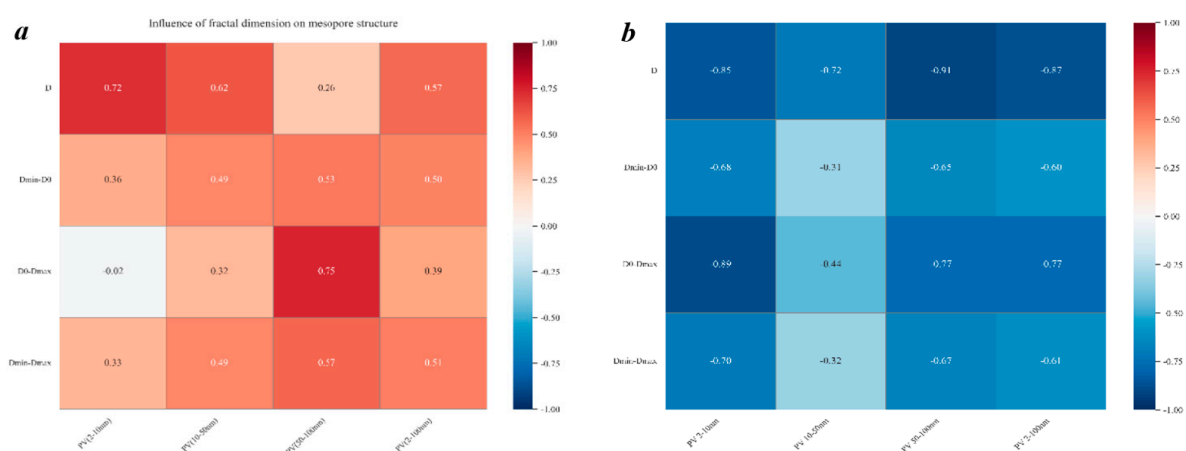


Figure 10. Correlation heat maps between fractal parameters and pore-structure parameters of Type I and Type II coal samples ((a), correlation heat map between fractal parameters and pore-structure parameters of Type I coal samples; (b), correlation heat map between fractal parameters and pore-structure parameters of Type II coal samples).

Figure 11a shows that pore volume in all pore-size intervals generally increases with increasing D . Among them, the 2–100 nm interval shows the largest slope, whereas the 10–50 nm interval exhibits a relatively good fitting relationship, indicating that total mesopore volume and medium-scale mesopores are more sensitive to variations in mono-fractal characteristics. Figure 11b further shows that pore volume in all pore-size intervals also increases with increasing $D_{min}-D_{max}$, and the correlations are relatively stronger for the 2–100 nm and 10–50 nm intervals. These results indicate that, in Type I, both mono-fractal and multifractal parameters are positively correlated with mesopore volume, particularly for medium-scale mesopores and the overall mesopore system.

In contrast, Figure 11c shows that pore volume in all pore-size intervals generally decreases with increasing D , and the fitting relationships are relatively stronger for the 50–100 nm and 2–100 nm intervals. Figure 11d further indicates that pore volume in all pore-size intervals also decreases overall with increasing $D_{min}-D_{max}$, with the most pronounced negative correlation occurring in the 50–100 nm interval. These results suggest that, in Type II, both mono-fractal and multifractal parameters are negatively correlated with mesopore volume, and that larger-scale mesopores and the overall mesopore system respond more strongly to changes in fractal characteristics.

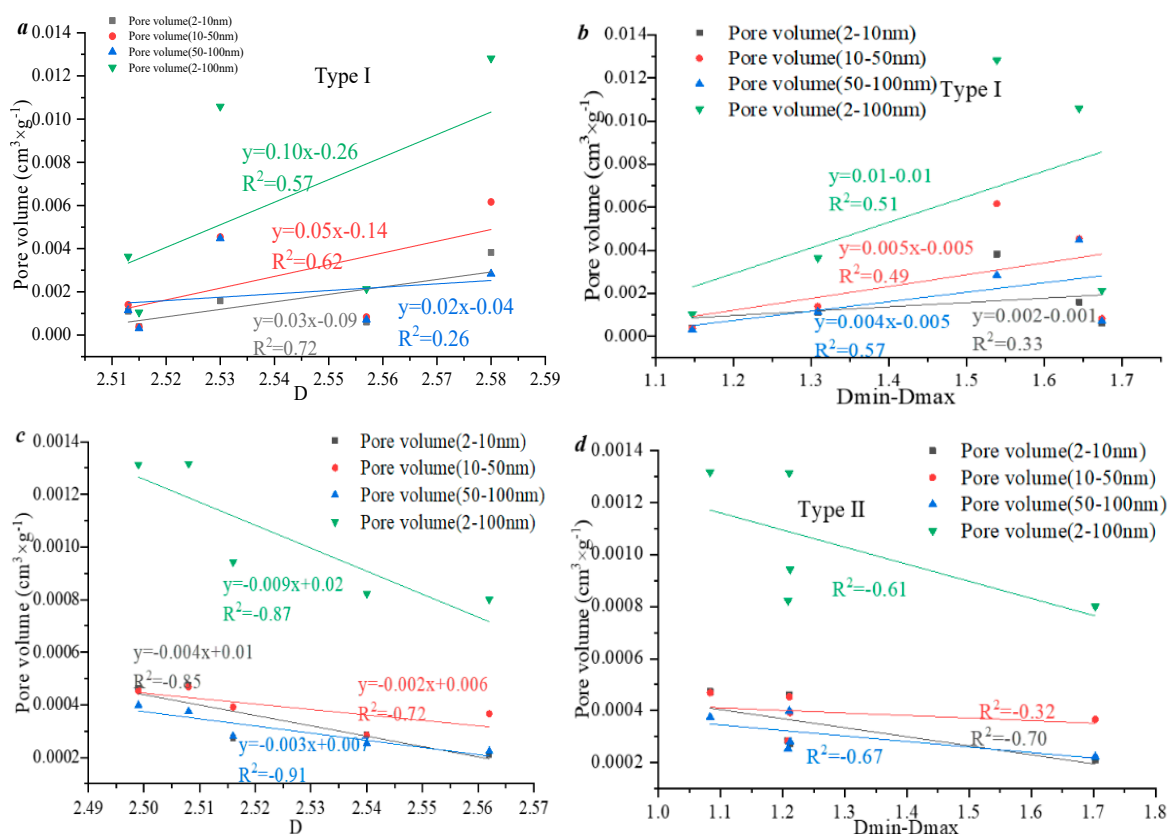


Figure 11. Fitting relationships between fractal parameters and pore volume in different pore-size intervals of Type I and Type II coal samples ((a), fitting relationships between mono-fractal dimension D and pore volume in different pore-size intervals of Type I coal samples; (b), fitting relationships between multifractal width $D_{\min} - D_{\max}$ and pore volume in different pore-size intervals of Type I coal samples; (c), fitting relationships between mono-fractal dimension D and pore volume in different pore-size intervals of Type II coal samples; (d), fitting relationships between multifractal width $D_{\min} - D_{\max}$ and pore volume in different pore-size intervals of Type II coal samples).

4. Conclusions

In summary, the present study compared mesopore structure and fractal characteristics of Xishanyao Formation coal samples with different maceral assemblages from the Nileke Depression, northeastern Yili Basin. The main conclusions are as follows:

- (1) The samples fall within a moderate maturity range, whereas vitrinite and inertinite contents vary widely. For comparison within this dataset, samples with vitrinite content $\geq 60\%$ were classified as Type I, and those with vitrinite content $< 60\%$ were classified as Type II. This grouping provides a practical basis for examining the relationship between maceral assemblages and pore characteristics.
- (2) Both sample types contain mesopores in the 2–100 nm range, but their pore-size distributions differ. Type I samples show a closer association between total mesopore volume and the 10–50 nm interval, whereas Type II samples show a closer association with the 50–100 nm interval. The two groups also differ in adsorption–desorption behavior and pore-distribution patterns.
- (3) Mono-fractal and multifractal parameters reflect these differences in pore organization. In Type I, medium-scale mesopores are more closely associated with pore-surface complexity and multiscale variation. In Type II, larger mesopores contribute more clearly to total pore-volume variation and heterogeneous pore distribution. Within the geological conditions of the Nileke Depression, these results suggest that maceral assemblages are related to mesopore organization and pore heterogeneity.

- (4) The findings are most directly applicable to the Xishanyao Formation coals in the study area. They may also provide a reference for other deep coal reservoirs with comparable coal rank, maceral composition, and geological history. However, the transfer of these conclusions to other basins should consider local depositional conditions, tectonic modification, mineral matter, and burial evolution.

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References

- Lu, F.; Liu, C.; Zhang, X.; Jia, B.; Wang, Y.; Liu, S.; Tang, Y.; Liu, J.; Lin, P. Study on full-scale pores characterization and heterogeneity of coal based on low-temperature nitrogen adsorption and low-field nuclear magnetic resonance experiments. *Sci. Rep.* **2024**, *14*, 16910. [[CrossRef](#)] [[PubMed](#)]
- Wang, H.; Wang, L.; Zheng, S.; Sun, Y.; Shen, S.; Zhang, X. Research on coal matrix pore structure evolution and adsorption behavior characteristics under different thermal stimulation. *Energy* **2024**, *287*, 129677. [[CrossRef](#)]
- Zhang, J.; Huang, H.; Zhou, W.; Sun, L.; Huang, Z. Study on Pore Structure of Tectonically Deformed Coals by Carbon Dioxide Adsorption and Nitrogen Adsorption Methods. *Energies* **2025**, *18*, 887. [[CrossRef](#)]
- Wang, J.; Liu, L.; Cui, Z.; Wang, H.; Li, T.; Duan, L.; Cheng, Y.; Su, P.; Li, M.; Wei, X. Multi-fractal characteristics of pore structure for coal during the refined upgrading degassing temperatures. *J. Pet. Explor. Prod. Technol.* **2021**, *11*, 2931–2942. [[CrossRef](#)]
- Ullah, B.; Cheng, Y.; Wang, L.; Yang, W.; Jiskani, I.M.; Hu, B. Experimental analysis of pore structure and fractal characteristics of soft and hard coals with same coalification. *Int. J. Coal Sci. Technol.* **2022**, *9*, 58. [[CrossRef](#)]
- Ma, Z.; Chen, Y.; Ma, D.; Li, G.; Li, W.; Ji, Y.; Zheng, C.; Wang, L.; Wang, X. Pore Fractal Characteristics of Different Macro-Coal Components and Influence on Adsorption/Desorption: A Case Study in the Huanglong Jurassic Coalfield. *ACS Omega* **2022**, *7*, 43770–43783. [[CrossRef](#)] [[PubMed](#)]
- Yao, Y.B.; Liu, D.M.; Tang, D.Z.; Tang, S.H.; Huang, W.H. Fractal characterization of adsorption-pores of coals from North China: An investigation on CH₄ adsorption capacity of coals. *Int. J. Coal Geol.* **2008**, *73*, 27–42. [[CrossRef](#)]
- Yao, Y.B.; Liu, D.M.; Tang, D.Z.; Tang, S.H.; Huang, W.H.; Liu, Z.H.; Che, Y. Fractal characterization of seepage-pores of coals from China: An investigation on permeability of coals. *Comput. Geosci.* **2009**, *35*, 1159–1166. [[CrossRef](#)]
- Cai, Y.D.; Liu, D.M.; Yao, Y.B.; Li, J.Q.; Liu, J.L. Fractal characteristics of coal pores based on classic geometry and thermodynamics models. *Acta Geol. Sin. (Engl. Ed.)* **2011**, *85*, 1150–1162. [[CrossRef](#)]
- Zhou, S.D.; Liu, D.M.; Cai, Y.D.; Yao, Y.B. Fractal characterization of pore–fracture in low-rank coals using a low-field NMR relaxation method. *Fuel* **2016**, *181*, 218–226. [[CrossRef](#)]
- Zhou, S.D.; Liu, D.M.; Cai, Y.D.; Yao, Y.B.; Che, Y.; Liu, Z.H. Multi-scale fractal characterizations of lignite, subbituminous and high-volatile bituminous coal pores by mercury intrusion porosimetry. *J. Nat. Gas Sci. Eng.* **2017**, *44*, 338–350. [[CrossRef](#)]
- Zhang, S.H.; Tang, S.H.; Tang, D.Z.; Huang, W.H.; Pan, Z.J. Determining fractal dimensions of coal pores by FHH model: Problems and effects. *J. Nat. Gas Sci. Eng.* **2014**, *21*, 929–939. [[CrossRef](#)]
- Mastalerz, M.; He, L.; Melnichenko, Y.B.; Rupp, J.A. Porosity of coal and shale: Insights from gas adsorption and SANS/USANS techniques. *Energy Fuels* **2012**, *26*, 5109–5120. [[CrossRef](#)]
- Yao, P.; Zhang, J.; Lv, D.; Vandeginste, V.; Chang, X.; Zhang, X.; Wang, D.; Han, S.; Liu, Y. Effect of water occurrence in coal reservoirs on the production capacity of coalbed methane by using NMR simulation technology and production capacity simulation. *Geoenergy Sci. Eng.* **2024**, *243*, 213353. [[CrossRef](#)]
- Zhao, J.; Tang, D.; Qin, Y.; Xu, H. Fractal characterization of pore structure for coal macro-lithotypes in the Hancheng area, southeastern Ordos Basin, China. *J. Pet. Sci. Eng.* **2019**, *178*, 666–677. [[CrossRef](#)]

16. Zhao, J.; Xu, H.; Tang, D.; Mathews, J.P.; Li, S.; Tao, S. A comparative evaluation of coal specific surface area by CO₂ and N₂ adsorption and its influence on CH₄ adsorption capacity at different pore sizes. *Fuel* **2016**, *183*, 420–431. [[CrossRef](#)]
17. Jiang, J.; Yang, W.; Cheng, Y.; Zhao, K.; Zheng, S. Pore structure characterization of coal particles via MIP, N₂ and CO₂ adsorption: Effect of coalification on nanopores evolution. *Powder Technol.* **2019**, *354*, 136–148. [[CrossRef](#)]
18. Zhang, J.; Wei, C.; Chu, X.; Vandeginste, V.; Ju, W. Multifractal analysis in characterizing adsorption pore heterogeneity of middle- and high-rank coal reservoirs. *ACS Omega* **2020**, *5*, 19385–19401. [[CrossRef](#)] [[PubMed](#)]
19. Wang, Z.; Wang, G.; Hao, C.; Hu, B.; Cheng, Y.; Liu, Z.; Qi, G. Study on multifractal of coal pore structure based on low-pressure argon adsorption and its effect on gas adsorption/desorption. *Energy Fuels* **2023**, *37*, 10915–10928. [[CrossRef](#)]
20. Lin, Y.; Qin, Y.; Ma, D.; Duan, Z. Pore structure, adsorptivity and influencing factors of high-volatile bituminous coal rich in inertinite. *Fuel* **2021**, *293*, 120418. [[CrossRef](#)]
21. Zheng, C.; Chen, Y.; Yu, L.; Lei, W.; Du, X.; Yang, F. Experimental investigation on pore characteristics of vitrain and durain in low-rank coal based on fractal theory. *Sci. Rep.* **2024**, *14*, 5008. [[CrossRef](#)] [[PubMed](#)]
22. Zhang, N.; Wang, S.; Wu, J.; Li, Z.; Wang, X. Full-scale pore structure characterization and its impact on methane adsorption capacity and seepage capability: Differences between shallow and deep coal from the Tiefa Basin in northeastern China. *Fractal Fract.* **2024**, *8*, 48. [[CrossRef](#)]
23. Zhang, Q.; Tang, S.; Zhang, S.; Xi, Z.; Xin, D.; Jia, T.; Yang, X.; Zhang, K.; Li, J.; Wang, Z. Methane adsorption capacity of deep buried coal seam based on full-scale pore structure. *Nat. Resour. Res.* **2025**, *34*, 1481–1505. [[CrossRef](#)]
24. Peta, K.; Kubiak, K.J.; Brown, C.A. Multiscale geometric analysis of dynamic wettability on complex, fractal-like, anisotropic surfaces. *Measurement* **2026**, *264*, 120328. [[CrossRef](#)]
25. Fu, H.J.; Tang, D.Z.; Xu, T.; Xu, H.; Tao, S.; Li, S.; Yin, Z.; Chen, B.; Zhang, C.; Wang, L. Characteristics of pore structure and fractal dimension of low-rank coal: A case study of Lower Jurassic Xishanyao coal in the southern Junggar Basin, NW China. *Fuel* **2017**, *193*, 254–264. [[CrossRef](#)]
26. Chen, S.; Tao, S.; Tang, D.; Xu, H.; Li, S.; Zhao, J.; Jiang, Q.; Yang, H. Pore structure characterization of different rank coals using N₂ and CO₂ adsorption and its effect on CH₄ adsorption capacity: A case in Panguan Syncline, Western Guizhou, China. *Energy Fuels* **2017**, *31*, 6034–6044. [[CrossRef](#)]
27. Miao, H.Y.; Veerle, V.; Zhang, J.J.; Chen, S.B.; Chang, X.C.; Du, Y.; Wang, Y.; Wei, C.T.; Luo, J.H.; Quan, F.K.; et al. Control mechanism of pressure drop rate on coalbed methane productivity by using production data and physical simulation technology. *Fuel* **2025**, *406*, 137060. [[CrossRef](#)]
28. Song, Y.; Jiang, B.; Li, F.; Liu, J. Structure and fractal characteristic of micro- and meso-pores in low- and middle-rank tectonically deformed coals by CO₂ and N₂ adsorption. *Microporous Mesoporous Mater.* **2017**, *253*, 191–202. [[CrossRef](#)]
29. Nie, B.; Liu, X.; Yang, L.; Meng, J.; Li, X. Pore structure characterization of different rank coals using gas adsorption and scanning electron microscopy. *Fuel* **2015**, *158*, 908–917. [[CrossRef](#)]
30. Teng, J.; Mastalerz, M.; Hampton, L. Maceral controls on porosity characteristics of lithotypes of Pennsylvanian high-volatile bituminous coal: Example from the Illinois Basin. *Int. J. Coal Geol.* **2017**, *172*, 80–94. [[CrossRef](#)]
31. GB/T 6848-2008; Method for the Determination of Maceral Group Composition and Vitrinite Reflectance in Coal (Determination of Maceral Group Composition and Vitrinite Reflectance of Coal). China Standard Press: Beijing, China, 2008.
32. GB/T 19587-2017; Determination of Pore Size Distribution and Porosity of Solid Materials by Gas Adsorption—Part 1: Principles and Procedures (Gas Adsorption Method for Pore Size Distribution and Porosity of Solid Materials). China Standard Press: Beijing, China, 2017.

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