



Article

Micro-CT-Based Pore Network Characterization and Microscopic Permeability Prediction Modeling for Deep Low-Rank Coal in the Tiefu Basin

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Abstract

Deep low-rank coal from the Daqiang Mine in the Tiefu Basin was investigated using micro-CT imaging with a voxel size of 1 μm . The CT-resolved connected macropore structures of 12 representative elementary volumes (REVs) were reconstructed, and corresponding equivalent pore network models were established. Steady-state, isothermal, single-phase continuum methane flow was simulated under prescribed inlet and outlet pressures with no-flow lateral boundaries, which primarily represent the flow capacity of CT-resolved connected macropores under unstressed conditions. The results showed that: (1) the S1 group exhibited a relatively compact pore structure, smaller throats, stronger spatial heterogeneity, and poorer connectivity, whereas the S2 and S3 groups contained better-developed and more highly connected pore–throat networks; (2) the simulated mean absolute permeabilities of the S1, S2, and S3 groups were 0.781, 0.969, and 0.910 mD, respectively. These values were generally close to, but slightly higher than, the experimental measurements, mainly because the digital models retained only CT-resolved connected pores and did not account for stress-induced compression or the flow-limiting effects of unresolved fine throats; (3) permeability was positively correlated with pore radius, throat radius, and coordination number, but negatively correlated with throat length, pore-to-throat ratio, tortuosity, and fractal dimension. Among these parameters, throat radius showed the strongest correlation with permeability; and (4) an empirical regression model was further established: $K = -4.809 + 0.672 r_t + 3.950 \tau$. The model exhibited a high goodness of fit ($R^2 = 0.952$, $p < 0.001$); however, its applicability is limited to the investigated coal samples from the Daqiang Mine. Overall, effective throat size and pore–throat connectivity provide more direct indicators of gas-transport capacity than total porosity alone, offering a pore-scale basis for identifying favorable CBM flow zones and optimizing reservoir stimulation strategies in the study area.



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Keywords: deep coal; pore structure; seepage simulation; permeability prediction model; micro-CT technology

1. Introduction

As the exploitable reserves in shallow areas gradually decrease, the extraction of deep coalbed methane has become a new research focus. Due to the complex geological

environment of deep formations, deep coal reservoirs' pore structure and permeability characteristics are distinct from the ones found in shallow coal reservoirs. They are more complicated [1]. Deep coal, as a porous medium with multi-scale pore and fracture structures, has pore structure characteristics that directly affect the macroscopic properties of the gas reservoir, with the macropore structure being a critical factor influencing seepage characteristics [2]. Therefore, conducting seepage characteristic simulations at the microscopic pore scale of macropore structures is extremely important for enhancing the extraction of deep coalbed methane.

In 1966, Hodot classified coal pores into four groups depending on the mechanical and permeability properties of coal: micropores (<10 nm), small pores (10–100 nm), mesopores (100–1000 nm), and macropores (>1000 nm), which remains the commonly used categorization standard for coal pore structures [3]. The methods for characterizing coal pore structures mainly fall into two categories. The first category is fluid intrusion methods, including N₂ and CO₂ adsorption experiments and mercury intrusion porosimetry (MIP) [4–8]. Combined with corresponding theoretical calculation methods, these experiments can obtain characteristics of the pore structure, including pore volume, specific surface area, and pore shape [9,10]. However, due to the limitations of the testing principles, they can only characterize pore structures within specific pore size ranges. The second category is photoelectric radiation techniques, which mainly include Field Emission Scanning Electron Microscopy (FE-SEM), X-ray Computed Tomography (CT), and Nuclear Magnetic Resonance (NMR) technology. Scanning electron microscopy can directly observe pore information on the sample surface, and depending on the selected resolution, it enables direct observation of pore structures with different pore sizes [11,12]. NMR technology not only characterizes pore structure features but also provides information on the fluid distribution within the sample [13–16]. CT technology, on the other hand, allows for three-dimensional reconstruction of the sample, and it has been widely used for the visualization and characterization of reservoir pore-fracture network structures [17–23]. Ni et al. [24] combined micro-CT scanning and image processing technology to establish a 3D structural model of macropores in coal and determined the throat radius and coordination number of the pore structure. Liu et al. [2] proposed an integrated characterization method based on CT 3D reconstruction, NMR T2 spectra, and Nuclear Magnetic Resonance Imaging (NMI). They conducted experiments on gas coal and anthracite samples, verifying the effectiveness of this method and studying the pore size distribution, porosity, and permeability features. Wang et al. [25] used 3D CT reconstruction, NMR experiments, and Magnetic Resonance Imaging (MRI) to study the seepage characteristics of coal seam water injection. They proposed a multi-scale, visual detection method for the seepage effect in coal and comprehensively characterized the water injection seepage effects in coal with different structures.

Gas migration in deep coal is a multiscale and coupled process. In addition to pressure-driven viscous flow through macropores and fractures, transport in submicron pores may involve gas slip, transition flow, and Knudsen diffusion. Gas pressure changes may also alter permeability through adsorption-induced swelling, desorption-induced shrinkage, and effective-stress-dependent closure of compliant pores and cleats. Researchers have conducted in-depth studies on gas seepage characteristics by combining numerical simulation methods with digital rock models established using CT technology, achieving significant results. Gerami et al. [26], using a pore network model based on CT 3D reconstruction, simulated methane flow in pore-fracture spaces. Wang et al. [27] and Zhou et al. [28], based on reconstructed coal structure models and using numerical simulation techniques, studied the seepage behavior of fluids in pores from a microscopic perspective and analyzed the impact of coal deformation on seepage. Johnson et al. [29] achieved the visualization of

microscopic seepage in coal macropores by comparing their simulations with experimental results. In the study of permeability models, Yuan et al. [30] established a coal permeability evolution model grounded in the equivalent characteristics of the dual-pore structure depending on the assumption of coal's dual-pore structure. They analyzed the impact of these equivalent characteristics on the evolution of coal permeability. Zhou et al. [11], through creep seepage experiments and theoretical models at different temperatures, revealed the evolution of coal permeability as influenced by temperature, matrix-fracture interactions, and creep deformation. Chang et al. [31] conducted spontaneous imbibition experiments on coal samples from the Qinshui, Ordos, and Zhungeer Basins in China, studying the resulting changes in matrix permeability and proposing a corresponding permeability model.

Coal is commonly regarded as a typical dual-porosity medium consisting of a low-permeability matrix pore system with high storage capacity and a highly conductive pore–fracture network [32,33]. Conventional dual-porosity models generally use storage and interporosity-flow parameters to describe fluid exchange between the matrix and fracture continua [34,35]. With the development of fractal theory, multiscale heterogeneity associated with pore- and fracture-size distributions, tortuous flow paths, and irregular fracture networks has been further incorporated into permeability models [36,37]. However, many existing models are still based on idealized capillary bundles or tree-like fracture networks and rely on structural parameters that are difficult to measure directly or calibrate accurately. In contrast, image-based pore network models can directly extract measurable geometrical and topological parameters, including pore and throat sizes, connectivity, coordination number, and tortuosity, from reconstructed three-dimensional pore spaces, thereby providing an important complementary approach for quantitatively elucidating the relationship between pore structure and permeability. Currently, most research on digital rock technology focuses on shallow coal seams, and due to limitations in instrument resolution, the pore sizes simulated are usually larger. Compared with shallow low-rank coal and deep medium- to high-rank coal, deep low-rank coal combines the relatively well-developed meso- and macropores and strong hydrophilicity and water sensitivity characteristics of low-rank coal with the effects of high in situ stress at depth, resulting in reduced effective pore connectivity and permeability, together with enhanced stress sensitivity and spatial heterogeneity. Deep coal reservoirs' pore and permeability characteristics are more complex, and there is relatively little research applying digital rock technology to low-porosity, low-permeability reservoirs for seepage characteristic studies. Regarding permeability model research, most models are based on macroscopic experimental parameters, lacking models considering the influence of pore structure parameters.

To address the above issues, high-resolution micro-CT imaging was employed to investigate the pore structure and flow characteristics of deep low-rank coal from the Tiefu Basin. A digital core model of the connected macropore structure with pore sizes greater than 1 μm was reconstructed, and a permeability prediction model applicable to deep low-rank coal in the Tiefu Basin was developed. The research framework comprised four main steps: (1) reconstructing the connected pore structure larger than 1 μm and establishing an equivalent pore network model; (2) quantitatively characterizing pore–throat geometry, connectivity, tortuosity, and fractal characteristics; (3) conducting pore-scale methane flow simulations using the digital core model; and (4) developing and validating a permeability prediction model incorporating multiple pore-structure parameters. This framework quantitatively links measurable geometrical and topological characteristics of the pore network to permeability, thereby providing a pore-scale basis for evaluating the fluid-flow capacity of deep coal reservoirs.

2. Materials and Methods

This section describes the sample preparation, laboratory porosity and permeability measurements, petrographic and proximate analyses, micro-CT scanning, image preprocessing and segmentation, local representative subvolume selection, pore-network extraction, and pore-scale permeability simulation.

2.1. Sampling

The experimental coal samples came from the Daqiang Coal Mine in the Tiefa Basin, Liaoning Province, from a working face at depths of 1100 to 1200 m within the research domain. After sampling, the samples were sealed in zip-lock bags and wax-sealed upon arrival at the surface. The geographical location of the Daqiang Coal Mine is shown in Figure 1. The coal samples' porosity and permeability were determined using the traditional core analysis techniques described in the Chinese national standard GB/T 29172-2012 [38]. Before porosity and permeability testing, all samples were dried at 105 °C to a constant weight. Based on Boyle's law, a helium porosimeter was used to test porosity, while gas permeability was measured using a CAT112 high- and low-permeability instrument (Coretest Systems Inc., Nashville, TX, USA). The samples were compressed at 200 psi while enclosed in a Hassler holder, and high-purity nitrogen was passed through the core samples to determine permeability. Table 1 displays the experimental coal samples' permeability and porosity characteristics.



Figure 1. Geographic map of the Daqiang coalmine.

Table 1. Statistical table of the test data of the coal samples.

No.	Ro, Max (%)	Porosity ϕ (%)	Permeability K (mD)	Proximate Analysis (%)				Coal Composition (%)			
				Mad	Aad	VMad	FCad	Vitrinite/Huminite	Inertinite	Exinite	Mineral
S1	0.62	4.14	0.754	6.03	3.46	38.97	51.54	86.07	7.21	4.22	2.50
S2	0.60	10.98	0.914	6.61	27.11	31.91	34.37	80.52	8.64	7.63	3.21
S3	0.63	11.70	0.858	6.98	21.78	35.58	35.66	84.61	8.62	3.48	3.29

2.2. Coal Petrographic Analysis

Coal petrology analysis is a crucial method for studying the origin, structure, composition, and physical–chemical properties of coal, and it is essential for understanding the features of coalbed methane reservoirs. This study tested the maceral composition and vitrinite reflectance ($R_{o, \max}$, %) of coal in the study area utilising a Leitz MPV-3 photometer microscope (Leitz, Wetzlar, Germany), in accordance with the Chinese national standards GB/T 6948-2008 [39] and GB/T 8899-2013 [40]. The evaluation of elements was conducted via a Vario-MICRO elemental analyzer (Elementar Analysensysteme GmbH, Langenselbold, Germany) in accordance with the Chinese national standard GB/T 19143-2017 [41]. The coal samples were analyzed using an SDTGA5000 industrial analyzer (Hunan Sundry Science and Technology Co., Ltd., Changsha, China) under air-dried conditions, following the ISO standard 17246-2010 [42] for proximate analysis, which was the applicable edition when the experiments were conducted. ISO 17246:2010 [42] has subsequently been superseded by ISO 17246:2024 [43]. The results of the coal petrology analysis for the experimental coal samples are displayed in Table 1.

2.3. CT Measurements

As a non-destructive testing technique, CT scanning can visually and precisely characterize the distribution of pores and fractures in three dimensions within coal samples. When conducting μ CT experiments, it is crucial to select appropriate sample sizes and resolution settings [28]. Deep coal typically exhibits low porosity and low permeability characteristics, with dominant pores being in the nanometer scale and fewer medium and large pores. Therefore, before conducting μ CT experiments, it is necessary to conduct MIP tests on the coal samples to obtain pore size distribution data, which can provide a basis for selecting CT samples and determining the appropriate resolution. The MIP experiment results show that deep coal exhibits a typical dual-pore structure, with the pore size distribution of micron-scale pores ranging from 1 to 1000 μ m. Considering the pore size distribution and the magnification of the CT equipment (2500 $\times$), this study selected cylindrical samples with dimensions of $\phi 2.9 \times 7.0$ mm, and the CT scan resolution was set to 1 μ m. The cylindrical geometry facilitates stable 360° rotation and specimen centering during scanning and avoids the sharp corners and abrupt variations in X-ray attenuation that may occur in prismatic samples, thereby reducing edge-related reconstruction artifacts. This study used a nanoVoxel-3000 series open-tube transmission high-resolution CT system (Sanying Precision Instruments Co., Ltd., Tianjin, China) for scanning. During the experiment, the ready-made samples of coal were fixed in the center of the CT machine's working turntable, and the sample height was adjusted to ensure that it was centered within the scanning area. A top-to-bottom scan was performed on the complete sample, with an exposure time of 120 s, and the total scanning time was 32 h. The final image resolution generated was 1 μ m.

2.4. Image Processing and Computation of Representative Elementary Volume (REV)

Upon acquiring the raw CT scan pictures, image preprocessing is required, and the image processing workflow is shown in Figure 2. The first step involves processing the CT slices, including image cropping, noise reduction filtering, threshold division, and 3D reconstruction. The three most important ones are threshold segmentation, 3D reconstruction, and filtering to reduce noise [23]. In this study, the median filtering method was chosen for noise reduction to eliminate various noises introduced during the CT scanning process and to obtain more accurate scan results. The Digital Terrain Model (DTM) threshold division technique was used for threshold segmentation. A CT image is essentially composed of numerous pixels with independent grayscale values, forming a

digital grayscale array. By treating the grayscale value of each pixel as an elevation value, each CT image can be regarded as a unique digital terrain model, which can be expressed by the following equation.

$$\varphi(x) = \frac{V_E}{V_T} = \frac{\sum_{r_i=0}^x (x - r_i)H(r_i)}{\sum_{r_i=0}^x xH(r_i)}, \quad (1)$$

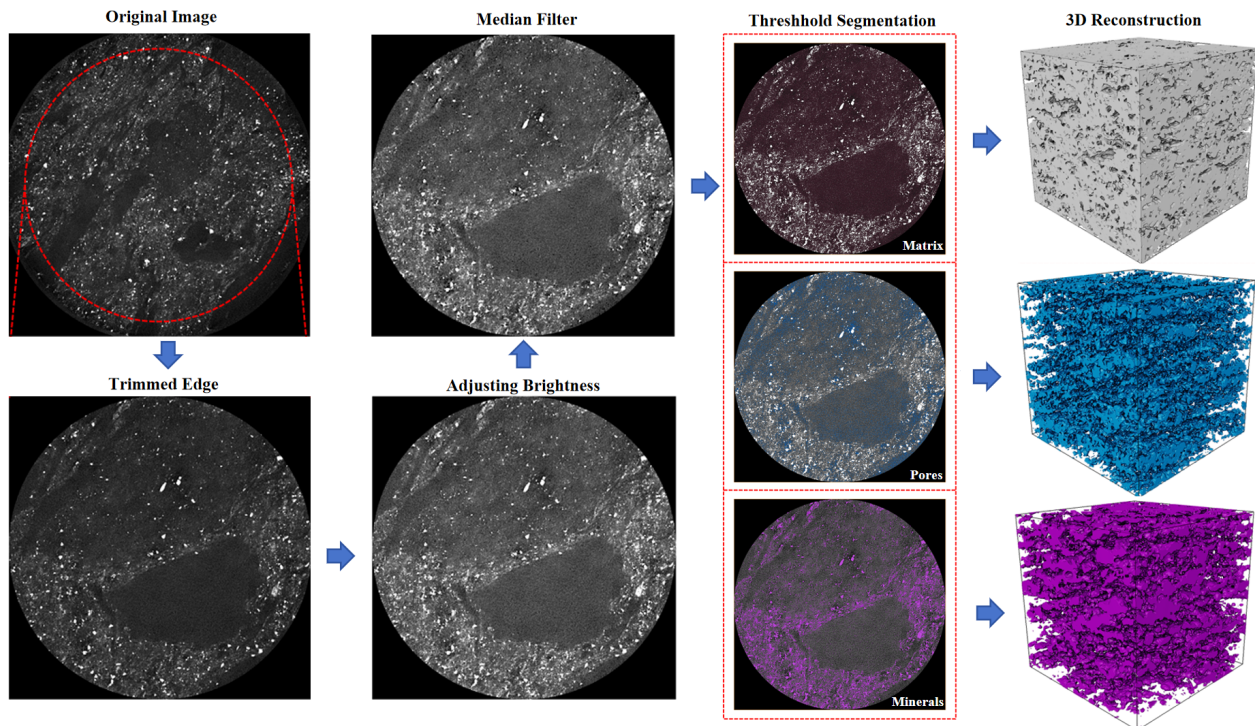


Figure 2. CT Image Processing and 3D reconstruction.

In the equation, $H(r_i)$ denotes the frequency corresponding to grayscale value r_i in the grayscale histogram over the range $[r_{max} - r_{min}]$; V_E is the pore volume; V_T is the total volume; v , is the volume of a single pixel or voxel; r_{max} and r_{min} are the maximum and minimum grayscale values in the image, respectively; and r_i is the grayscale value of an individual pixel.

The idea behind this technique is to create a digital terrain model using the greyscale values of each location in the CT scan, and then create a function that varies among porosity and greyscale values. The threshold for the CT picture is established by finding the extremum of this function. At the image segmentation stage, a reasonable threshold is directly related to the visualization quality and the accuracy and authenticity of the characterization of the microscopic pore and fracture structures in the coal. This study selected the appropriate threshold based on the grayscale value distribution features of the coal matrix, pores, and minerals in the CT images during the visualization and characterization process. Finally, the 3D reconstruction of the components was achieved using Avizo software 2020.1 [18].

Due to computational power limitations, it is generally challenging to perform 3D reconstruction of pore structures and subsequent analysis on the entire CT image dataset. Therefore, selecting a Representative Elementary Volume (REV) from the complete dataset is necessary. When choosing the REV, both computational resources and the precision of the reconstruction's findings must be considered. The commonly used method for assessing the measurement of the REV is calculating the porosity of the Region of Interest (ROI). When the porosity becomes stable as the ROI size increases, meaning it no longer

undergoes significant changes, the REV at this scale is considered to accurately represent the coal sample's macroscopic physical characteristics [32]. The final calculated REV size is $160 \times 160 \times 160$ voxels, as Figure 3 illustrates. In this study, 12 REV samples were selected (each sample being $160 \times 160 \times 160$ voxels). The S1 group includes samples S1-1, S1-2, S1-3, and S1-4; the S2 group includes samples S2-1, S2-2, S2-3, and S2-4; and the S3 group includes samples S3-1, S3-2, S3-3, and S3-4.

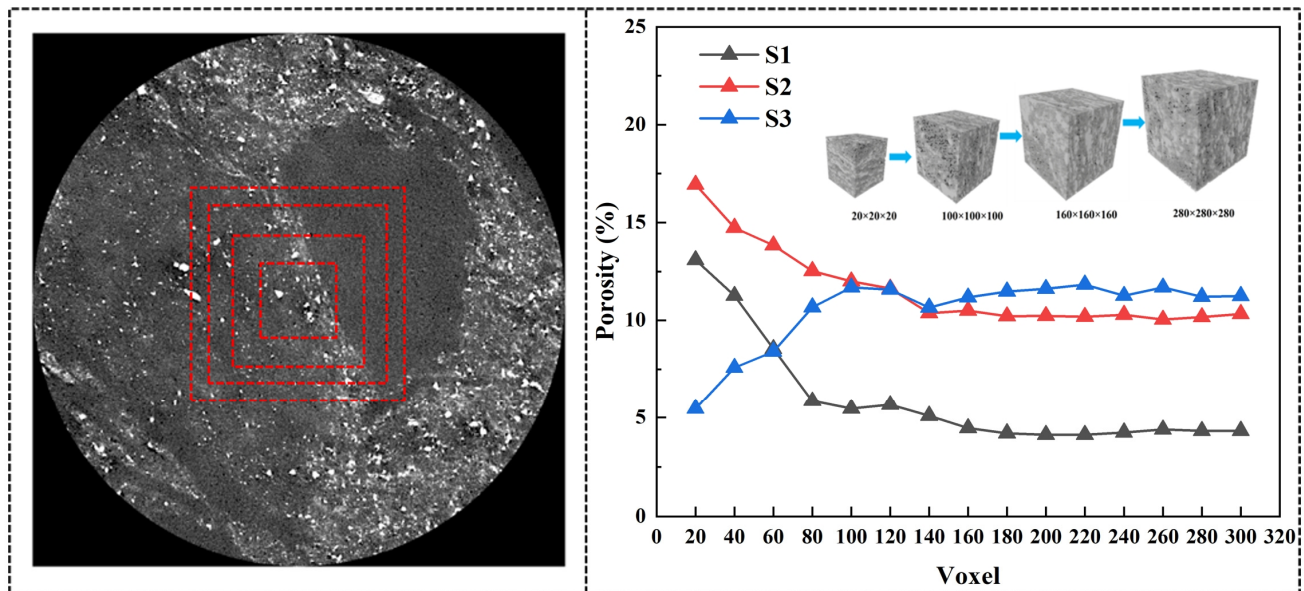


Figure 3. Relationship between porosity and different ROI sizes.

3. Results

3.1. Coal Characteristics

Table 1 presents the coal petrology characteristic parameters of the experimental samples. The experimental coal samples' $R_{o, \max}$ falls between 0.60% and 0.63%, demonstrating that the coal rank belongs to low-rank coal. The highest maceral content is vitrinite, followed by inertinite and liptinite, with the lowest content being minerals. The moisture, ash, volatile matter, and fixed carbon contents range from 6.03% to 6.98%, 3.46% to 27.11%, 31.91% to 38.97%, and 34.37% to 51.54%, respectively, indicating that the deep coal in Daqiang is characterized by high moisture, high volatile matter, and low fixed carbon content. The porosity and permeability of the experimental coal samples were in the range of 4.14% to 11.70% and 0.754 to 0.914 mD, respectively, with average values of 8.94% for porosity and 0.842 mD for permeability, classifying them as low-porosity and low-permeability reservoirs.

3.2. Quantitative Analysis of Pore Net Work Model

Quantitatively evaluating the size features of pores and throats is crucial for the safe and efficient generation of deep coalbed methane. The pores in coal can be classified into two categories depending on connectivity: connected pores and isolated pores. Connected pores denote all the pores associated with the pore network, serving as the primary channels for gas migration and playing a pivotal role in influencing coal seam permeability. On the other hand, isolated pores are dispersed pores that are unconnected to the pore network, and their contribution to gas flow is minimal. Therefore, this section focuses on extracting connected pores based on the REV pore structure and establishing the corresponding Pore Network Model (PNM).

The principle of constructing a PNM is to represent pores and throats using a geometric model, where spheres represent the pores and tubes represent the throats. The spatial positions and sizes of the spheres and tubes correspond to the actual positions and dimensions of the pores and throats, respectively [32]. This simplified PNM can intuitively and precisely illustrate the spatial distribution and morphological features of the internal pore structure in coal. It is beneficial for studying the dynamic changes in permeability during coalbed methane extraction. The specific process for constructing the PNM is as follows: First, the “Axis Connectivity” module is used to process the connectivity of the pores in the REV, identifying the connected pores within the coal body. Next, the “Separate Objects” module separates and labels the connected pores based on the connectivity relationships between neighboring voxels. Different colors distinguish the segmented pores. Finally, an equivalent PNM with the morphological and topological structure of the pores is generated. The detailed model construction process is shown in Figure 4. On this basis, pore structure properties including porosity, pore radius, throat radius, throat length, coordination number, pore-to-throat ratio, and tortuosity can be further extracted. These parameters provide essential data for analyzing the mechanisms affecting coalbed methane permeability. The specific pore structure properties of the experimental samples are displayed in Table 2.

As shown in Table 2, the porosity ranges from 3.525% (S1-3) to 14.129% (S3-1), averaging 8.740%. The pore radius ranges from 3.484 μm (S1-3) to 7.872 μm (S2-2), having a 6.089 μm mean pore radius. The throat radius distribution ranges from 1.128 μm (S1-3) to 1.781 μm (S2-1), averaging 1.459 μm . The throat length ranges from 13.602 μm (S2-2) to 27.176 μm (S1-3), with a mean value of 18.77 μm . The pore throat ratio varies from 2.744 (S2-2) to 6.588 (S1-3), with a mean value of 4.094. The coordination number varies from 4.984 (S1-3) to 7.719 (S3-3), averaging 6.045. The tortuosity ranges from 1.137 (S2-2) to 1.196 (S1-3), with an average value of 1.171.

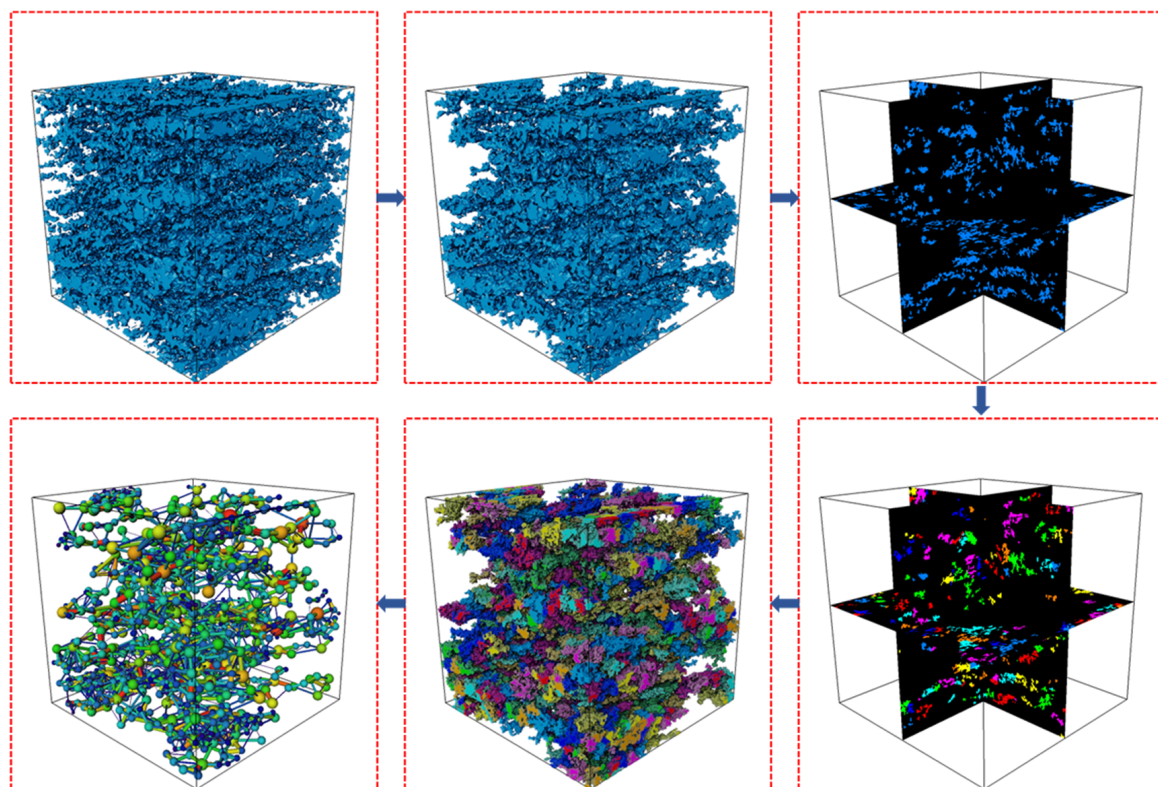


Figure 4. Schematic of Pore Net Work model extraction.

Table 2. Pore structure parameters of digital core model.

Number	Porosity (%)	Pore Radius (μm)	Throat Radius (μm)	Throat Length (μm)	Pore-Throat Ratio	Coordination Number	Tortuosity
S1-1	5.151	5.332	1.329	18.097	3.557	5.589	1.173
S1-2	4.093	5.100	1.277	17.080	4.234	5.298	1.191
S1-3	3.525	3.484	1.128	27.176	6.588	4.984	1.196
S1-4	4.142	5.878	1.476	20.393	3.982	6.049	1.173
S2-1	9.197	6.927	1.781	13.893	2.766	6.347	1.145
S2-2	11.395	7.872	1.726	13.602	2.744	6.895	1.137
S2-3	10.204	6.892	1.756	13.864	2.787	6.811	1.141
S2-4	10.123	6.762	1.334	21.327	5.478	5.615	1.187
S3-1	14.129	5.869	1.444	22.045	4.718	6.310	1.186
S3-2	12.134	6.077	1.313	23.105	5.011	5.901	1.180
S3-3	11.113	6.847	1.691	16.418	3.531	7.719	1.166
S3-4	10.082	5.403	1.477	15.576	3.304	5.820	1.177

As shown in Table 3, based on the combined N_2 adsorption, MIP, and CT results, the total pore volumes of samples S1, S2, and S3 were 0.023, 0.048, and 0.050 $\text{cm}^3 \cdot \text{g}^{-1}$, respectively, indicating that the pore systems of S2 and S3 were more developed than that of S1. Significant differences were observed among the pore-size fractions. S1 was dominated by micropores, with a micropore volume of 0.016 $\text{cm}^3 \cdot \text{g}^{-1}$, accounting for 70.51% of the total pore volume, whereas mesopores and macropores contributed only 16.15% and 13.35%, respectively. In contrast, S2 was dominated by mesopores, which exhibited a pore volume of 0.029 $\text{cm}^3 \cdot \text{g}^{-1}$ and accounted for 60.90% of the total pore volume. The pore-size distribution of S3 was relatively balanced, with micropores, mesopores, and macropores accounting for 33.05%, 32.95%, and 34.00%, respectively; among them, the macropore volume was the highest at 0.018 $\text{cm}^3 \cdot \text{g}^{-1}$.

Table 3. Full aperture Pore structure parameters of tested samples.

Sample No.	$V_{\text{total}}/(\text{cm}^3 \cdot \text{g}^{-1})$	Volume/($\text{cm}^3 \cdot \text{g}^{-1}$)			Volume Ratio/(%)		
		V_1	V_2	V_3	V_1	V_2	V_3
S1	0.023	0.016	0.004	0.003	70.51	16.15	13.35
S2	0.048	0.011	0.029	0.007	23.59	60.9	15.51
S3	0.050	0.016	0.016	0.018	33.05	32.95	34.00

Comparative analysis reveals that the S1 group has relatively low porosity, smaller pore radius, and smaller throat radius but longer throat length, higher pore throat ratio, and more significant tortuosity. The pore structure of the S1 group is more complex, with a winding fluid flow path, which restricts the smooth movement of fluid through the pore network, resulting in lower permeability. In contrast, the S2 group shows higher porosity, a larger pore radius, and a relatively larger throat radius. The throat length is shorter, with the lowest pore throat ratio, and the coordination number is relatively high, with the lowest tortuosity. The pore structure of the S2 group is more consistent, with good connectivity among pores and throats, allowing for smoother fluid flow paths, leading to significantly higher permeability than the S1 group. The S3 group has porosity and pore radius values between the S1 and S2 groups, with moderate throat radius and longer length. The pore-to-throat ratio is intermediate, and the coordination number is relatively high, with S3-3 having a coordination number of 7.719. Although the pore structure of the S3 group is relatively complex, the fluid flow path is pretty smooth, and its permeability is between that of the S1 and S2 groups, showing a moderate level of permeability. In summary, the pore structure features of different samples significantly impact permeability.

The S2 group exhibits the best pore connectivity and the highest permeability, while the S1 group's complex structure and higher tortuosity result in lower permeability. The S3 group falls in between, demonstrating moderate permeability.

3.3. Pore Size Distribution (PSD) Quantitative Parameter Statistics

Figure 5 displays the quantitative PSD results for pore radius, throat radius, throat length, and coordination number obtained through the equivalent PNM. According to Figure 5, the pore-size distribution exhibits an apparent unimodal pattern within the CT-resolvable pore-size range, while the peak at approximately 2.5–4.0 μm may be influenced by the imaging resolution. The pore radius of S1-1 is mainly concentrated between 2 and 3 μm , with a peak at 2.5 μm . There are 282 pores in this category, which makes up 63% of the overall amount of pores. S2-1's dominant pore size is distributed between 3 and 4 μm , while the dominant pore size of S3-1 is between 2.5 and 3.5 μm , corresponding to 58% and 61% of the overall amount of pores, respectively. The pore size distribution range of S2-1 and S3-1 is more prominent, indicating that their pore structures are more favorable for fluid storage and transport. Regarding throat radius, the throat radius of S1-1 is mainly concentrated around 1.2 μm , while S2-1 and S3-1 have relatively larger throat radii, primarily focused at 1.5 μm and 1.4 μm , respectively. Specifically, throats with a radius of 1.5 μm in S2-1 account for 66% of the overall quantity of throats, while in S3-1, throats with a radius greater than 1.3 μm constitute 61% of the entire amount. In addition, the throat length of S1-1 is relatively short, mainly concentrated around 20 μm , while the throat lengths of S2-1 and S3-1 are concentrated at 40 μm and 30 μm , respectively. The coordination number, as an important parameter for measuring pore connectivity, reflects the degree of connectivity between pores. Pores with low coordination numbers (such as isolated pores possessing a coordination number of 0) enhance gas storage but minimally facilitate fluid flow. An elevated coordination number signifies an increased number of connecting channels between pores, enhancing fluid mobility. As shown in Figure 5, in S1-1, 89% of the pores have a coordination number below 8. In contrast, the coordination numbers of S2-1 and S3-1 are significantly higher, especially in S3-1, where the coordination number is mainly concentrated around 10. In summary, the pore structure of S1-1 is denser, with smaller throat radii and poorer connectivity, leading to weaker permeability. On the other hand, the dominant pore and throat structures in S2-1 and S3-1 exhibit higher connectivity and permeability, further validating the analytical findings of their pore structure characteristics.

Surface porosity can visually reveal the two-dimensional distribution characteristics of the internal pore structure in the samples, identify pore variation patterns across different slices, and provide insights into the uniformity, connectivity, and distribution of local pore clusters within the samples. This holds substantial importance for comprehending the permeability of the samples. In this study, based on the extracted REV, slice analysis was performed along the XY plane at intervals of 1 voxel in the Z-axis direction, and the surface porosity was calculated layer by layer. Figure 6 shows the surface porosity distribution trends for each sample.

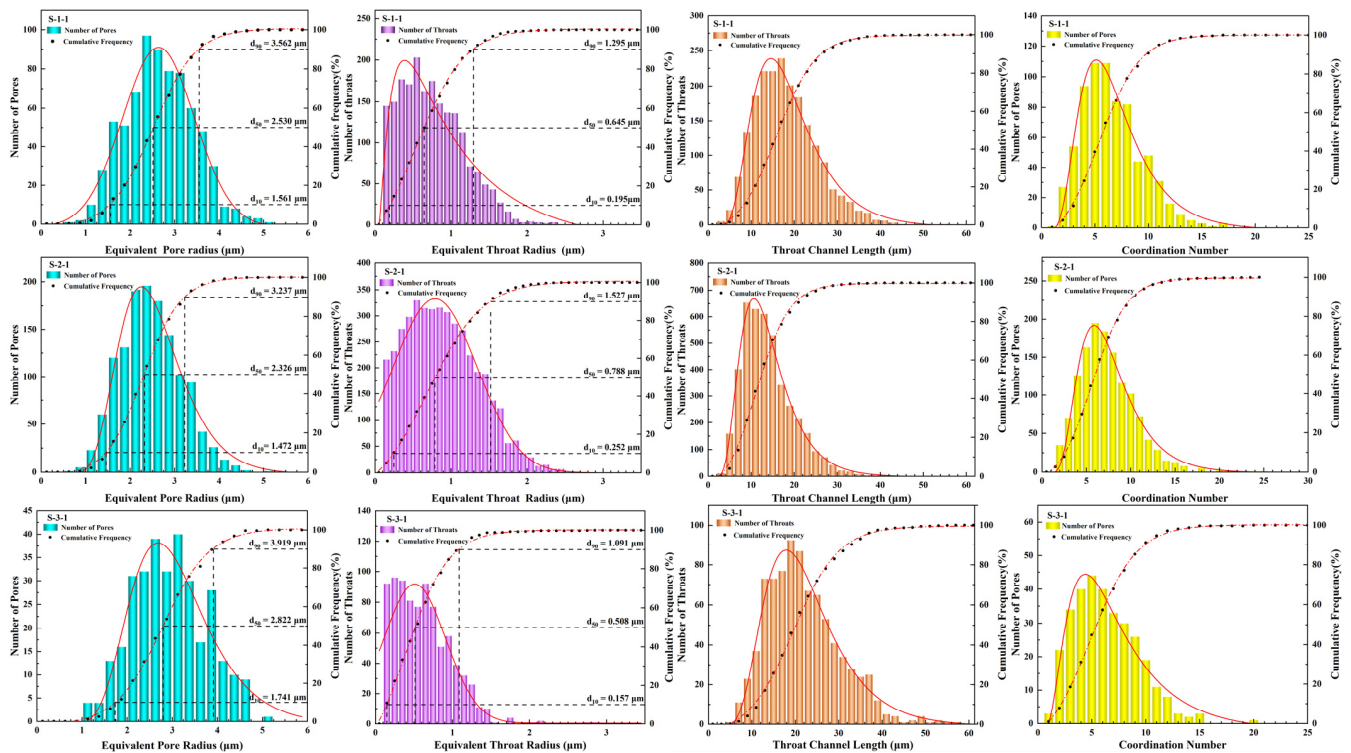


Figure 5. Distribution of pore radius, throat radius, throat length, and coordination number based on digital core model (S1-1, S2-1, and S3-1).

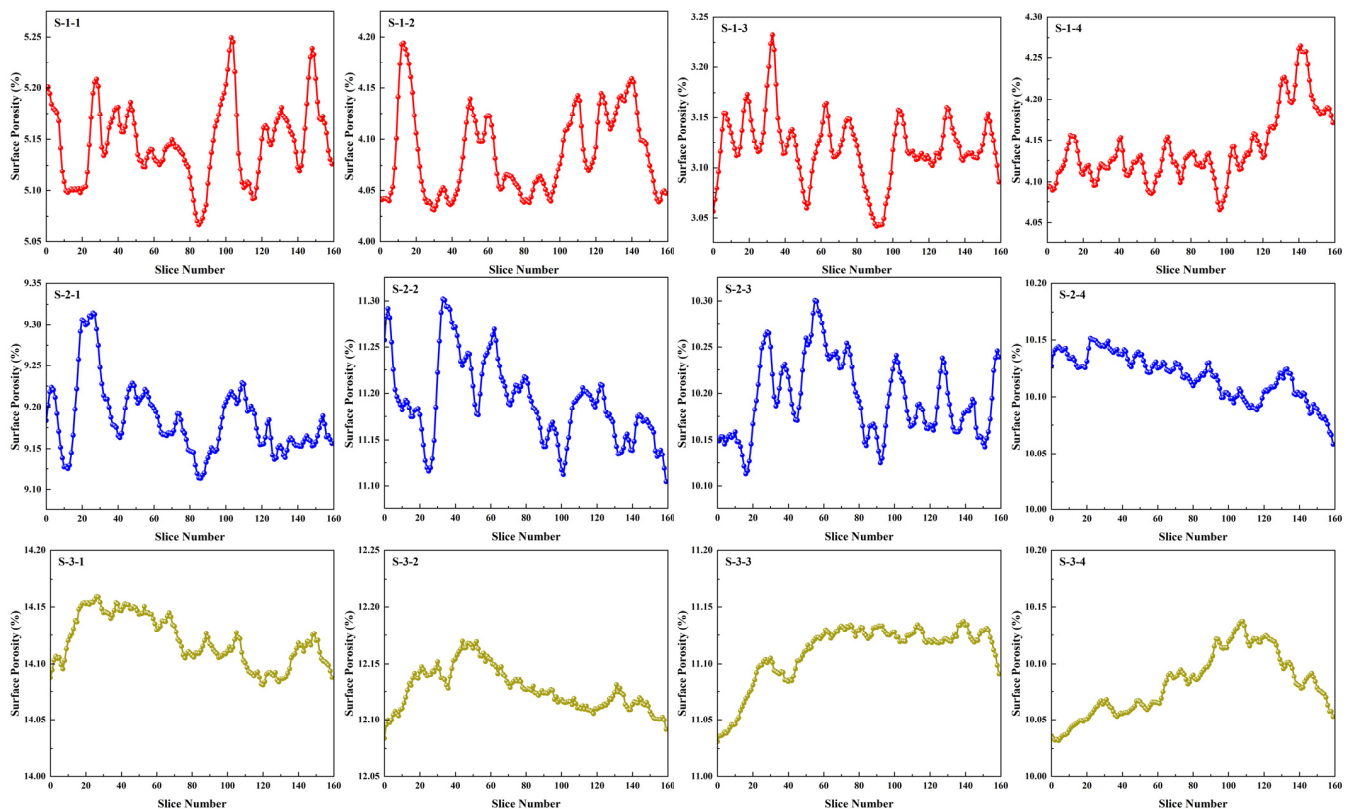


Figure 6. Surface porosity distribution of tested sample.

As shown in Figure 6, the porosity of the S1 group samples fluctuates significantly, indicating a complex pore structure with multiple large pore clusters. In sample S1-1, the porosity peaks between 0 and 110 μm , with values ranging from 5.15% to 5.25%, suggesting

the presence of large pore clusters in this region. S1-2 and S1-3 show similar porosity trends, rising first and then falling, with peak values around 90 μm and 110 μm , where the porosity reaches 5.25% and 3.25%, respectively, indicating large pore clusters at these locations. In contrast, S1-4 shows relatively smooth porosity fluctuations, suggesting a more uniform structure without large pore clusters. The S2 group samples exhibit localized, more significant fluctuations. In S2-1, the porosity peaks multiple times between 20 and 90 μm , with values ranging from 9.0% to 9.5%, indicating the presence of several pore clusters in this region. In S2-2, the porosity decreases first and then increases, with peaks at 40 μm and 120 μm , where the porosity reaches 11.5% and 11.0%, respectively. S2-3 also shows multiple fluctuations, with maximum values at 30 μm and 100 μm , reaching 10.5% and 10.8%, respectively. On the other hand, S2-4 exhibits an overall decreasing trend with small fluctuations, indicating a more uniform pore distribution without significant pore clusters. In comparison, the porosity changes in the S3 group samples are the most stable. In S3-1, the porosity fluctuates between 14.0% and 14.2%, indicating a relatively uniform pore structure. The porosity in S3-2 ranges from 12.0% to 12.2%, showing overall stability. The fluctuations in S3-3 and S3-4 are small, with porosity values between 11.5% to 11.8% and 11.0% to 11.3%, respectively, indicating that these two samples also have uniform pore structures without significant large pore clusters. Based on data digitally extracted from the slice-wise surface porosity curves, the coefficients of variation for porosity in all 12 REV models were below 1%, indicating generally minor porosity fluctuations along the slicing direction within each model. The CV values of the S1 group ranged from 0.63% to 0.91%, noticeably higher than those of the S2 group (0.20–0.41%) and the S3 group (0.16–0.28%), suggesting that the S1 group exhibited relatively stronger spatial heterogeneity in pore structure, whereas the S3 group showed greater overall homogeneity.

4. Discussion

4.1. Model Set-Up and Boundary Conditions

In the pore structure of coal, connected pores serve as the primary conduits for fluid movement and contribute significantly to the permeability of CBM. However, experimental methods typically focus on the entire coal sample, making it challenging to examine the seepage characteristics of connected pores. Before conducting the simulations, we calculated the Reynolds numbers (Re) for the selected coal samples along different flow directions, which ranged from 0.005 to 0.293. Most values were below the critical Reynolds number, indicating that the simulated flow conditions in this study were within the laminar-flow regime.

Building upon the previously constructed equivalent PNM, this section will conduct pore-scale seepage simulations to analyze fluid flow through the connected pores. The specific simulation process follows: derived from the constructed pore network model using the “Generate Pore Network Model” command, the “Absolute Permeability Experiment Simulation” command in the XLab Hydro module is used to start the absolute permeability experiment simulation. During the simulation, fluid viscosity can be set, and the “Set Pressure Inlet” and “Set Pressure Outlet” commands are used to define the inlet and output pressures together with the flow direction. This setup allows for numerical simulation of fluid flow under different pressure gradients. The boundary conditions for this section are set as follows: the seepage direction is the flow along the Z-axis through the pore space. There is no slip of the fluid within the pore space, and the entire pore space is in a sealed and isolated state, with no fluid entering from outside or exiting the internal space. The pressure gradient is set as the boundary condition, with the inflow and outflow ends of the pore model defined by establishing the inlet pressure at 1.1 MPa and the outlet pressure at 0.1 MPa. The convergence criterion is set to 0.0001, and the number of iterations is set to a

minimum of 1000 and a maximum of 1,000,000, as illustrated in Figure 7. After these settings are completed, the simulation is run using the “Run Simulation” command to calculate fluid flow through the sample’s pore structure. The “Absolute Permeability Experiment Simulation” command derives the sample’s absolute permeability grounded in Darcy’s law. Once the simulation is complete, the “Measure Permeability” command can be used to view and export the permeability calculation results. The simulations were designed to calculate the intrinsic permeability of the CT-resolved connected macropore network. The fluid was treated as a steady, single-phase Newtonian continuum, and the coal skeleton was assumed to be rigid. No-slip conditions were imposed at solid–fluid interfaces. The four lateral surfaces were assigned no-flow boundary conditions, whereas the two surfaces normal to the Z-axis were defined as the pressure inlet and outlet. Gas adsorption and desorption, Klinkenberg slip, Knudsen diffusion, unresolved nanopores, sub-voxel surface roughness, and stress-induced deformation were not explicitly considered.

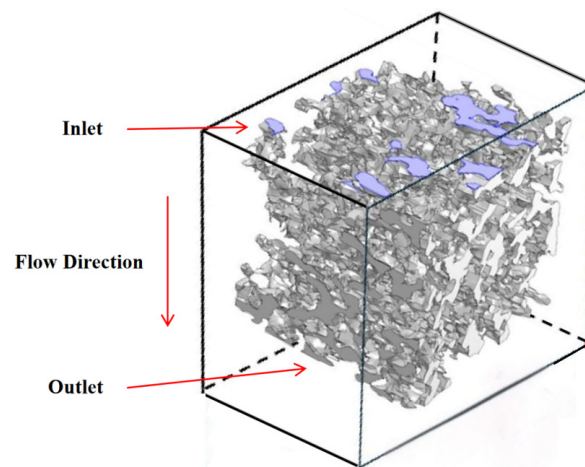


Figure 7. Settings of boundary condition.

Darcy’s law is expressed as shown in Equation (2) [32]:

$$\frac{Q}{A} = -\frac{k\Delta p}{\mu L}, \quad (2)$$

where Q is the overall flow rate via the porous medium (m^3/s); A is the cross-sectional area of the fluid flowing through the sample (m^2); k is the absolute permeability (m^2); Δp is the pressure gradient given to the sample (Pa), L is the length of the sample in the flow direction (m), μ is the dynamic viscosity of the fluid ($\text{Pa}\cdot\text{s}$).

4.2. Absolute Permeability Calculation

Figure 8 shows the visualization of fluid flow paths for the experimental samples (S1-1 to S3-4). Different colors and lines represent the fluid flow trajectories within the pore structures, with red streamlines indicating the highest flow velocity and purple streamlines indicating the lowest flow velocity. As illustrated in Figure 8, the streamlines in the S1 group samples display more complex and winding paths, especially in S1-1 and S1-3, where the flowlines exhibit noticeable branching and detouring. This indicates that there are many narrow channels and disconnected regions within the pore space of this group, making the fluid flow paths more complicated. The fluid velocity exhibits significant variation across different regions. In the S1 group samples, due to the more complex pore structure, the fluid encounters more resistance when passing through narrow channels, reducing velocity. In contrast, the liquid flows more quickly in larger pore cluster areas. The streamlines in the S2 group samples show more uniform and continuous patterns, forming smoother flow paths

within the pore network. Especially in samples S2-2 and S2-3, the streamlines are tighter, indicating that these samples have better pore connectivity. The fluid can traverse the pore network with less obstruction, resulting in a relatively even flow velocity distribution. Due to the excellent connectivity of the pore structures, the fluid experiences less resistance in the S2 group samples, leading to more stable overall flow velocity with more minor variations in speed. The streamlines in the S3 group samples also exhibit good connectivity. The streamlines are continuous and evenly distributed, indicating that fluid flow within these samples is smoother. In particular, in S3-1 and S3-3, the variation in streamlines is minimal, suggesting that the pore spaces in these samples provide stable flow channels with good network connectivity. The fluid can move relatively freely through the pore network. Overall, the fluctuation in flow velocity is slight, indicating that these samples have good pore connectivity and low flow resistance.

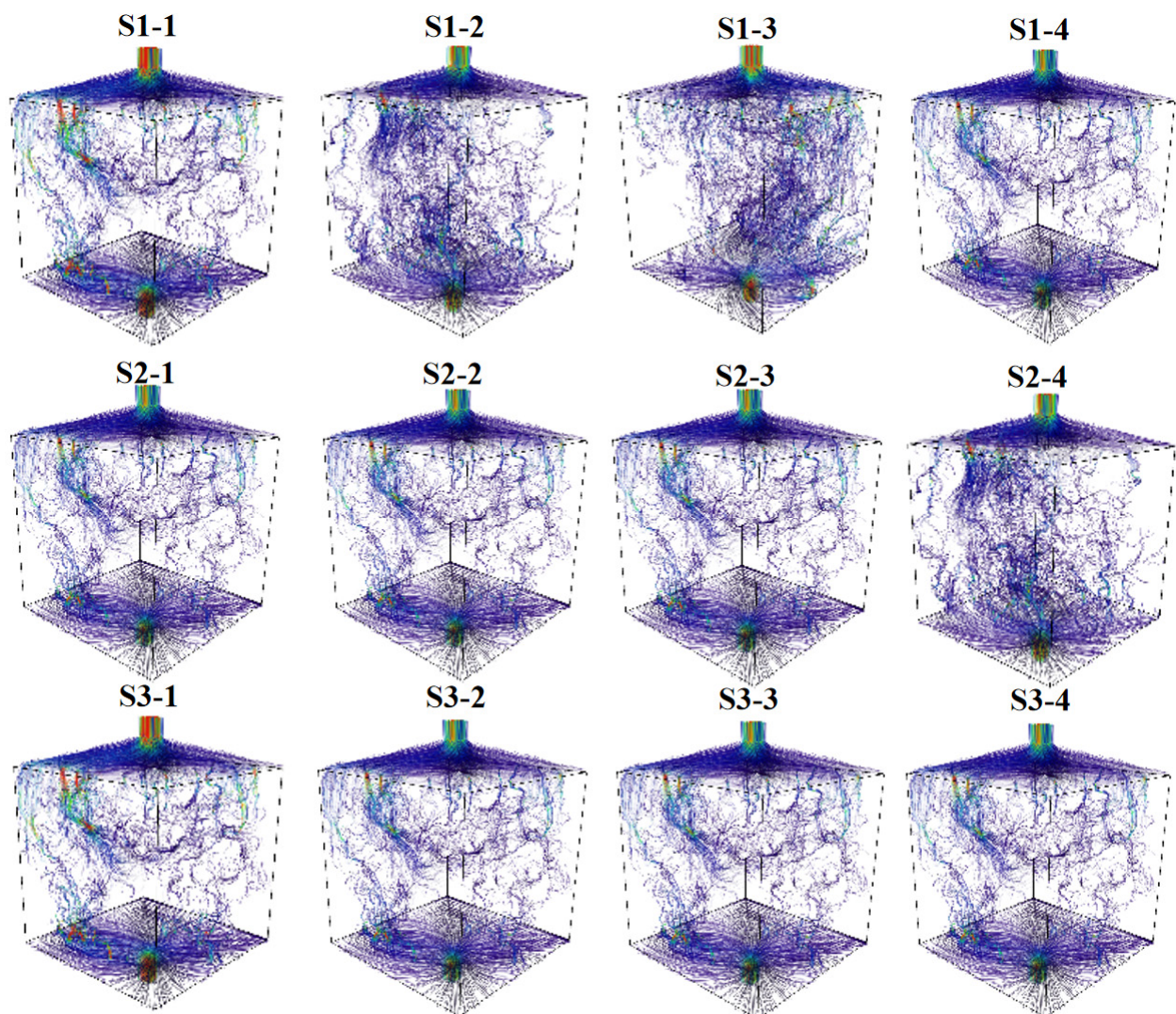


Figure 8. Distributions of streamlines for tested sample.

Table 4 presents the calculated absolute permeability results for the experimental samples. As shown in Table 4, the average computed permeability for the S1 group is 0.781 mD, while the experimental permeability is 0.754 mD. For the S2 group, the average calculated permeability is 0.969 mD, with the experimental permeability being 0.914 mD. The S3 group has an average calculated permeability of 0.910 mD, while the experimental permeability is 0.858 mD. Overall, the experimental permeability is slightly lower than the calculated permeability. This is because the calculated values are based on a connected

pore model, while in experiments, the presence of isolated pores affects gas mobility. Despite this, the difference between the calculated and experimental permeability values is slight, indicating that the calculation method effectively simulates the permeability of the samples. This validates the accuracy and effectiveness of the technique used for permeability calculation.

Table 4. Calculation Results of Absolute permeability for tested samples.

No.	Permeability (mD)	Average Calculated Permeability (mD)	Experimental Permeability (mD)
S1-1	0.783	0.781	0.754
S1-2	0.776		
S1-3	0.604		
S1-4	0.961		
S2-1	1.006	0.969	0.914
S2-2	1.044		
S2-3	1.003		
S2-4	0.824		
S3-1	0.926	0.910	0.858
S3-2	0.740		
S3-3	1.034		
S3-4	0.937		

4.3. Correlation Between Pore Structure Parameters and Permeability

Figure 9 presents the correlation analysis between pore structure parameters and absolute permeability. There is no discernible relationship between porosity and permeability, as Figure 9a illustrates. This is because permeability is influenced by porosity and other factors including pore connectivity, throat radius, and throat length. As previously discussed, the S1 group samples have a complex pore structure with poor connectivity, which results in relatively low permeability. Figure 9b shows a positive correlation between pore radius and permeability, with a correlation coefficient of 0.649. A larger pore radius implies lower resistance for fluid flow, allowing more fluid to pass through and reducing frictional resistance during flow, increasing permeability. Figure 9c demonstrates a strong positive correlation between throat radius and permeability, with a correlation coefficient as high as 0.871. Throats are the narrow channels connecting pores, and a larger throat radius leads to lower resistance for fluid passage. According to Poiseuille's law, the throat radius to the fourth power determines the fluid flow rate. Therefore, an increase in throat radius significantly reduces flow resistance, greatly enhancing permeability. As shown in Figure 9d, A negative association of 0.615 is found between throat length and permeability. Longer throats extend the fluid flow path, increasing frictional resistance during flow and causing more energy loss. Consequently, permeability decreases as throat length increases. In Figure 9e, permeability and the pore throat ratio show a negative relationship, with a correlation coefficient of 0.680. The ratio of pore radius to throat radius is known as the pore throat ratio. A higher ratio indicates a more significant size difference amongst pores and throats. When fluid flows from a large pore into a much smaller throat, flow resistance increases significantly, reducing permeability. Figure 9f illustrates the positive correlation between coordination number and permeability, with a correlation coefficient of 0.715. The pore network's connectedness can be seen in the coordination number. A higher coordination number means more connecting paths between pores, allowing fluid to flow more easily. This reduces the resistance in any single flow path, increasing permeability. Figure 9g shows that tortuosity has a negative correlation with permeability, exhibiting a correlation value of 0.592. Tortuosity represents the degree of complexity in the fluid's flow

path through the pore space. A higher tortuosity indicates that the fluid must navigate more winding paths, increasing flow resistance and energy loss, which leads to lower permeability. Finally, as depicted in Figure 9h, the fractal dimension negatively correlates with permeability, with a coefficient of 0.540. The fractal dimension is a crucial indicator of the intricacy of the pore structure. An elevated fractal dimension indicates a more intricate and heterogeneous pore structure, making the fluid flow path more convoluted and irregular, increasing flow resistance and reducing permeability.

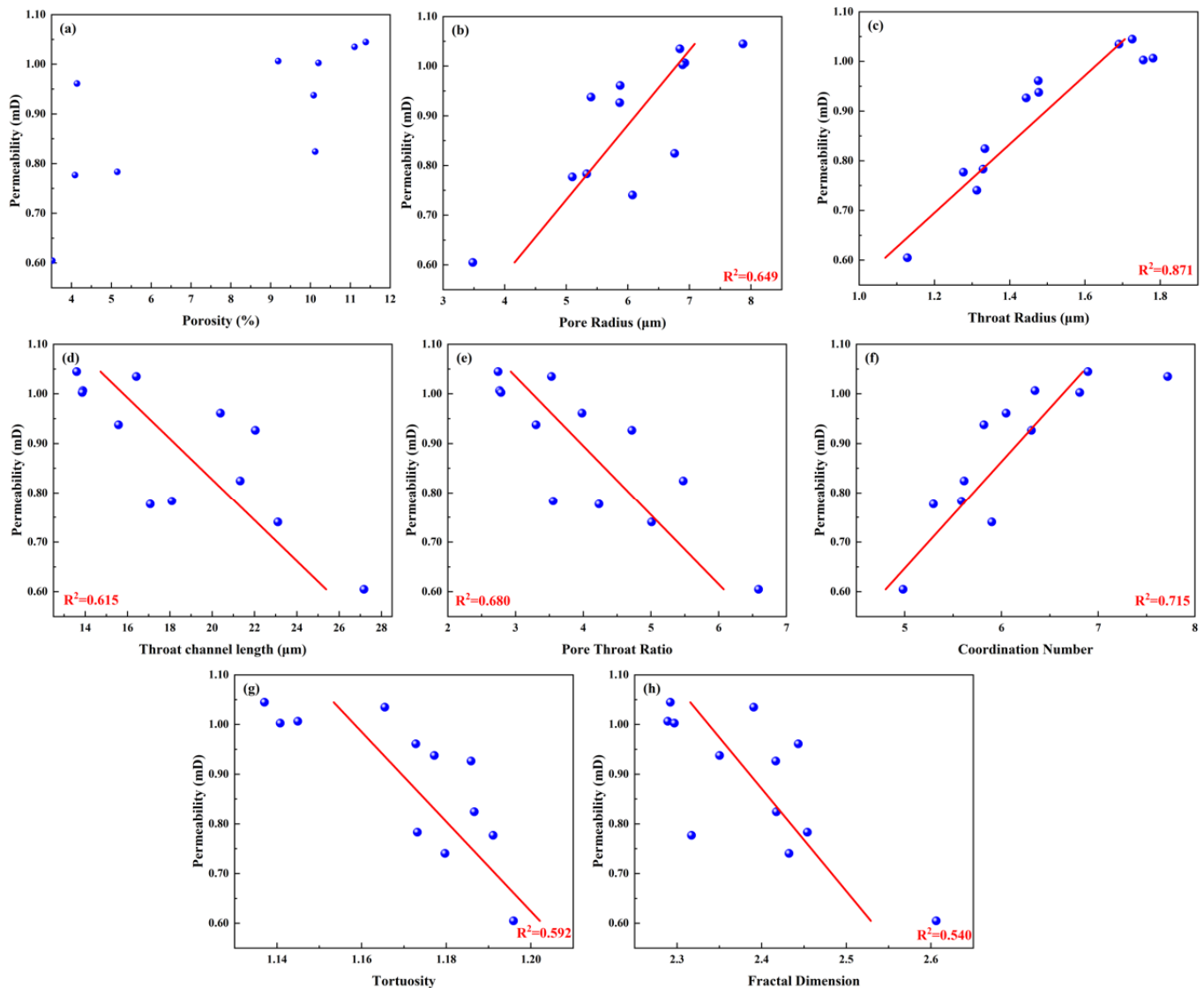


Figure 9. Correlation between permeability and pore structure parameters.

In summary, the relationships between pore structure parameters and permeability show different trends, indicating that the factors influencing permeability are complex. Throat radius and coordination number are the key positive factors affecting permeability, while throat length, pore throat ratio, tortuosity, and fractal dimension significantly negatively impact permeability. Longer throats increase viscous dissipation and reduce conductance. A high pore-to-throat ratio indicates that large pores are connected by narrow throats, producing repeated contraction and expansion and increasing local pressure losses. Greater tortuosity increases the effective transport distance and viscous energy loss. A higher fractal dimension in the present intact coal samples reflects stronger geometric irreg-

ularity and heterogeneity, which reduces the proportion of the pore network contributing effectively to through-flow.

4.4. Permeability Prediction Model

Multiple factors with complex interaction mechanisms influence the permeability of deep coal reservoirs. As previously discussed, permeability significantly correlates with pore and throat radius, pore-to-throat ratio, coordination number, and other pore structure parameters. The influencing mechanisms have been simplified in this study to quantitatively study the influence of these factors on permeability by assuming that each linearly independent factor has a linear correlation with permeability. This assumption established a multiple linear regression model that comprehensively considers the effects of various pore structure parameters on permeability. Multiple linear regression models analyze the relationship between several independent variables and a dependent variable and use statistical methods to construct a mathematical model for predicting the value of the target variable.

This model uses regression analysis to quantify the impact of different independent variables on permeability and improves prediction accuracy through training and optimization [14]. Before establishing the multiple linear regression model, a multicollinearity diagnosis of the independent variables is required to eliminate potential multicollinearity issues [13]. The multicollinearity diagnosis results indicate no significant multicollinearity among the pore structure parameters. Based on the correlation analysis results from Section 4.3, throat radius, coordination number, pore throat ratio, pore radius, throat length, and tortuosity were selected as the primary factors influencing permeability. SPSS statistical 27 software was used to conduct multiple linear regression analysis, resulting in the establishment of a multiple linear regression model for permeability, as shown in Equation (3):

$$K = a + br_t + cCN + dP_T + er_p + fL_t + g\tau, \quad (3)$$

where K is the permeability; r_t is the throat radius; CN is the coordination number; P_T is the pore throat ratio; r_p is the pore radius; L_t is the throat length; τ is the tortuosity; a is the constant; b, c, d, e, f, g are the coefficients corresponding to the respective pore structure parameters.

Before the calculation, all variables must be standardized to eliminate the effects of dimensions and units. The standardized variables are then input into the SPSS software, with permeability as the dependent variable, to perform multiple linear regression analysis.

The model parameters are solved using the least squares method, and significance tests are conducted for the model and its parameters. The correlation coefficient of the model is 0.952, indicating that the model has significant statistical relevance. Among the pore structure parameters, throat radius and tortuosity statistically impact permeability ($p < 0.05$). Therefore, after excluding variables with severe multicollinearity and statistically insignificant effects, the final multiple linear regression model for permeability was established as follows:

$$K = -4.809 + 0.672 r_t + 3.950 \tau, \quad (4)$$

Eight REV models ($160 \times 160 \times 160$ voxels), labeled S1–S8, were selected from the original CT dataset to develop the multiple linear regression model. An additional six REV models of the same size, labeled T1–T6 and not included in model development, were used to independently evaluate the predictive performance of the model. Table 5 presents the pore structure parameters and absolute permeability of these samples.

Table 5. Pore structure parameters of tested samples.

No.	Mean Porosity (%)	Mean Pore Radius (μm)	Mean Throat Radius (μm)	Mean Throat Length (μm)	Mean Co-ordination Number	Mean Pore-Throat Ratio	Mean Tortuosity	Experiment Value (mD)	Predicted Value (mD)
S1	4.182	2.325	1.471	14.159	2.978	4.287	1.191	0.870	-
S2	3.189	2.385	1.546	14.675	3.073	5.470	1.178	0.931	-
S3	5.192	2.554	1.785	16.432	3.339	6.371	1.159	0.951	-
S4	9.194	2.483	1.915	10.685	3.046	7.116	1.185	1.164	-
S5	11.182	2.466	1.724	15.813	3.408	5.339	1.178	1.037	-
S6	12.183	3.017	1.713	20.537	4.172	6.179	1.172	0.940	-
S7	11.335	4.086	1.552	23.215	2.86	5.934	1.223	1.057	-
S8	10.435	5.921	1.953	44.673	4.375	5.777	1.192	1.224	-
T1	5.151	5.332	1.329	18.097	3.557	5.589	1.173	0.783	0.721
T2	4.093	5.100	1.277	17.080	4.234	5.298	1.191	0.777	0.758
T3	9.197	6.927	1.781	13.893	2.766	6.347	1.145	1.006	0.915
T4	10.123	6.762	1.334	21.327	5.478	5.615	1.187	0.824	0.780
T5	14.129	5.869	1.444	22.045	4.718	6.310	1.186	0.926	0.850
T6	12.134	6.077	1.313	23.105	5.011	5.901	1.180	0.740	0.738

Figure 10 shows the comparative analysis between experimental permeability and predicted permeability. The figure's red line represents the ideal case where the predicted results perfectly agree with the experimental results. Based on the analysis of Figure 10, the predicted results align well with the experimental data, indicating that the established model can effectively predict the permeability of deep coal reservoirs and demonstrates high reliability.

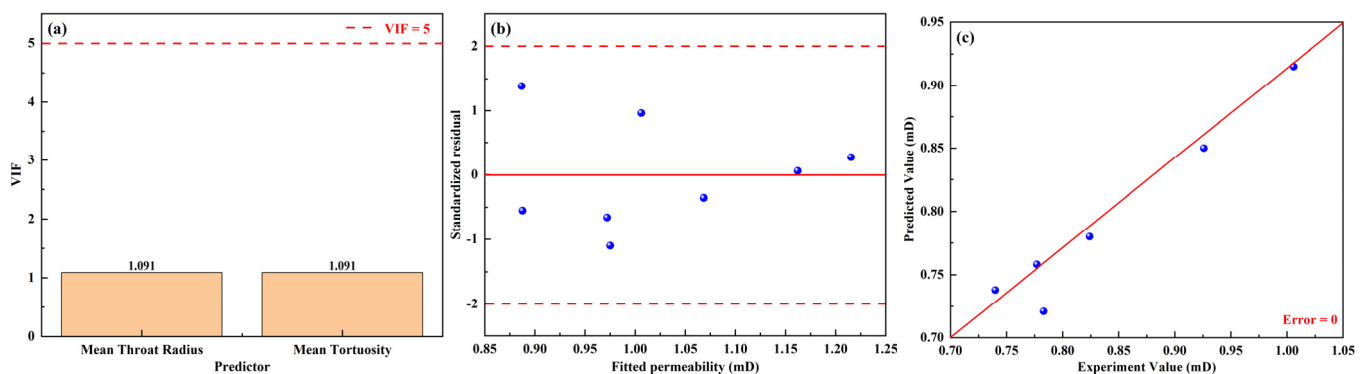


Figure 10. Diagnostic results for the permeability regression model: (a) variance inflation factors (VIF) of the retained predictors, (b) standardized residuals versus fitted permeability values, (c) Scatter plots of permeability obtained from centrifugal experiments and those from the mathematical model.

The reduced regression model was statistically significant ($F(2, 5) = 49.098$, $p < 0.001$, with $R^2 = 0.952$). The mean absolute error, root-mean-square error, and mean absolute percentage error were 0.0213 mD, 0.0253 mD, and 2.21%, respectively. The VIF values of both predictors were 1.091, indicating no meaningful multicollinearity.

5. Conclusions

This study utilized CT technology to construct a digital rock model of the macropore structure in deep coal from the Daqiang mine. Pore structure parameters and distribution curves for connected pores were obtained. Pore-scale seepage simulations were performed applying the equivalent pore network model, and absolute permeability was calculated. Based on the examination of the relationship between pore structure parameters and permeability, a multiple linear regression model was created, comprehensively taking into account how various pore structure parameters affect permeability. The following are the primary findings:

- (1) The investigated coal is characterized by low porosity and permeability, high moisture content, and high volatile-matter content. The reconstructed digital cores represent CT-resolved connected macropores.
- (2) Pronounced differences in pore–throat structure and flow capacity were observed among the samples. The S1 group exhibited smaller throats and poorer connectivity, whereas the S2 and S3 groups contained better-developed and more connected pore–throat networks. Throat size and connectivity are therefore important indicators of gas-transport potential in deep coal reservoirs.
- (3) The simulated mean absolute permeabilities of the S1, S2, and S3 groups were 0.781, 0.969, and 0.910 mD, respectively. The numerical results were generally close to, but slightly higher than, the experimental values because the digital models retained only CT-resolved connected pores and did not account for fine throats, local blockage, or effective-stress-induced deformation.
- (4) Permeability generally increased with pore radius, throat radius, and coordination number, but decreased with throat length, pore-to-throat ratio, tortuosity, and fractal dimension. Throat radius showed the strongest correlation with permeability, indicating that effective throat size and continuity are more important to gas transport than total porosity alone. Reservoir evaluation and stimulation should therefore prioritize well-connected dominant flow pathways.
- (5) The multiple linear regression model based on mean throat radius and mean tortuosity describes the statistical relationships between CT-derived macropore parameters and permeability for the REV samples investigated. However, it remains an empirical, sample-specific model applicable only to the tested coal from the Daqiang Mine. The positive partial coefficient of tortuosity may reflect coupling or suppression effects within the small dataset and should not be interpreted causally.
- (6) This study is limited by the small sample size, single-mining-area dataset, and CT resolution, and it does not incorporate effective stress, adsorption–desorption, matrix deformation, slip flow, or Knudsen diffusion. Future work should include larger and more diverse datasets, multiscale pore characterization, and independent validation under different stress conditions to develop coupled stress–adsorption–flow permeability models.

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