Research Article

Reconstruction of 3D Micro Pore Structure of Coal and Simulation of Its Mechanical Properties

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This article takes the low permeability coal seam in the coalfield of South Judger Basin in Xinjiang, as a research object. The pore structure characteristics of coal rock mass in low permeability coal seam were analyzed quantitatively using scanning electron microscopy (SEM) through the methods of statistics and digital image analysis. Based on the pore structure parameters and the distribution function of the coal rock mass, a three-dimensional porous cylinder model with different porosity was reconstructed by FLAC3D. The numerical simulation study of reconstructed pore model shows that (1) the porosity and the compressive strength have obvious nonlinear relation and satisfy the negative exponential relation; (2) the porosity significantly affects the stress distribution; with the increase of micro porosity, the stress distribution becomes nonuniform; (3) the compressive failures of different models are mainly shear failures, and the shape of fracture section is related to porosity; (4) the variation of seepage coefficient of the pore reconstruction model is consistent with the development of micro cracks. The micro mechanism of the deformation and failure of coal and the interaction of multiphase flow with porosity are revealed, which provides a theoretical reference for the clean development of the low permeability coal seam.

1. Introduction

With the adjustment of China's energy structure and the increasing demand for clean mining, exploring the intrinsic relationship between the coal pore structure and macro and micro mechanical properties has significant theoretical meaning for solving mining and other fields of engineering problems, such as prefracturing of coal seams, coal bed methane mining, underground coal gasification, and unconventional oil and gas resources [1–4].

Domestic and foreign scholars pay much attention to the study of the relationship between the micro structure of coal seam and its macro and micro mechanical properties. Firstly, the pore structure of the coal seam is the reservoir space and also the spatial of the gas-liquid flow [5, 6], which is the main factor that affects the coal gas storage capacity and the seepage characteristics. The pore structure of coal

has a direct influence on the gas adsorption and desorption characteristics [7]. Secondly, the study of the characteristics of the micro pore structure is helpful for analyzing the influence of pore structure on the crack propagation, coal bed methane, and gas outburst [8, 9], which are helpful for the prediction of coal seam gas resources and coal and gas outburst risk.

At present, the acquisition and analysis of the pore structure characteristics, the macroscopic mechanical properties, and the deformation and failure behavior of coal and rock mass mainly depend on the methods of field sampling and indoor experiment and numerical simulation. The relationship between porosity and compressive strength and shear strength of sandstone is studied [10]. Hatzor and Palchik [11] probed into the effect of the porosity of dolomite on the crack stress intensity of rock uniaxial compressive strength and fracture and gave an empirical relationship between porosity and stress intensity. The discrete element model

FIGURE 1: SEM images of coal sample before and after magnification.

is used to study the relationship between stress and strain, acoustic emission characteristics, strain localization, and shear reinforcement [12]. The three-dimensional statistical model of rock pore structure is constructed, and the influence of the pore on the stress distribution, the failure mode, and the fracture connectivity of rock are analyzed [13]. The three-dimensional pore model is established and the influence of pore structure parameters on the mechanical properties of porous sandstone is discussed [14]. Based on the model of micro pore structure of rock, the inner mechanism of the physical and mechanical behavior of rock is analyzed [15]. The relationship between pore structure parameters and physical and mechanical properties of coal and rock mass is studied, and an empirical relationship model is established for evaluation, classification, and prediction of physical parameters [16]. Most scholars study the change of macroscopic properties of the coal and rock mass, by experimental means, which can only indirectly reflect the effect of pore structure on the physical and mechanical properties. But the quantitative analysis of the internal mechanism between the coal pore structure and macroscopic physical and mechanical properties is less. On the basis of statistical analysis, the three-dimensional pore reconstruction model provides a new approach for the quantitative study of the mechanism of pore structure parameters of coal rock.

Based on the above analysis, selecting the typical low permeability coal seam in the coalfield of South Judger Basin in Xinjiang as the research object, we constructed a three-dimensional cylinder pore model of low permeability. We analyze the influence of the distribution law of micro pores on the physical and mechanical properties of the low permeability coal rock using the numerical simulation method.

2. Pore Structure Parameter Test

The experiment was made with the low permeability coal seam in the coalfield of South Judger Basin in Xinjiang, and the pore structure characteristics of low permeability coal seam were obtained by scanning electron microscope. Using Otsu threshold banalization processing method [17], SEM image of coal samples under different magnification is processed (Figure 1) and pore structure parameters, such

FIGURE 2: Pore diameter distribution.

as pore diameter, number, location, spacing, and statistical properties, are extracted. A large number of CT and SEM experiments show that the number of pores satisfies an approximate uniform distribution along the circumference, and the pore space and pore size are in normal distribution and exponential distribution [18–20].

According to the SEM data of coal samples, the pore statistical model with different porosity is established. The pore distribution in pore statistical model is uniform and the pore size distribution is exponential distribution. The pore size distribution function is expressed as

$$f(r) = A \times \exp(-Br) + C, \quad (1)$$

where A , B , C are constants and r is the aperture. The diameter of the image is calculated, and the ratio of the number of apertures to the total aperture is calculated (Figure 2).

The circle is divided into 25 equal intervals. If the number of holes in each interval is in uniform distribution, the following should be satisfied:

$$f(x) = \frac{1}{25 - 0} = 0.04, \quad (0 \leq x \leq 25). \quad (2)$$

FIGURE 3: Pore number distribution.

TABLE 1: Pore coordinates and aperture.

Numbers	Pore coordinates	Pore diameter
1	(22.33, 7.25)	0.66
2	(14.80, 4.81)	2.57
3	(9.52, 6.92)	3.12
4	(0, 24.49)	1.49
5	(6.99, 21.51)	0.71
6	(−4.59, 14.14)	8.18
7	(−8.74, −2.84)	7.22
8	(−0.76, −0.55)	0.96
9	(4.85, −3.53)	5.35
10	(23.27, −7.5607)	0.84
⋮	⋮	⋮

The number of pores in the processed image is calculated, and the numerical value of the ratio of the number of pores distributed in different circumferential intervals to the total number of pores is obtained. The specific distribution of pore number is shown in Figure 3.

For a given specimen height section of the pore, according to the plane polar coordinates method to determine the location of its pores, the statistical function of pore coordinate is expressed as

$$P(\rho \cos \theta, \rho \sin \theta), \quad (0 \leq \rho \leq 25, 0 \leq \theta \leq 360^\circ). \quad (3)$$

The partial coordinate information of pores on the circumferential surface in the $Z = 50$ mm direction is shown in Table 1.

3. Three-Dimensional Model of Pore Structure

According to the statistics derived from the pore position, number, size parameters, and the distribution function, using the Monte Carlo method, simulated annealing algorithm, and Matlab program, two groups of number series consisting of the parameters and distribution function are generated [21, 22]. Each row of the 3-column random sequences in accordance with the characteristics of uniform distribution

represents the three-dimensional coordinates of each pore, where two groups of one-row and multiple-columns random number sequence, accordingly, represent the random distribution of pore diameter. At the same time, the number of pores can be determined according to the measured porosity and pore size distribution, and the distribution of the number of pores can meet the regularity of the uniform distribution.

Because the space position of the pore, pore size distribution, and the number of changes are random, the difficulty of the finite element program exists in the grid, element size, and quantity control, so FLAC3D is chosen to construct the pore model. Considering the limitation of minimum size of the unit of FLAC program, scale-up of pore radius obtained in the experiment was made, at the same time keeping the porosity and porosity distribution unchanged and thus making the model and the actual coal samples have good geometric similarity.

Importing the generated random number series into the FLAC3D through the self-compiled program and, then, using FISH language, a three-dimensional cylinder is built by pore model with a diameter 50 mm, height 100 mm, and maximum pore radius 3.6 mm (Figure 4).

4. Numerical Simulation of Uniaxial Compression of Three-Dimensional Pore Reconstructed Models

The numerical simulation of the uniaxial compression of the 3D reconstruction model with different pores was carried out in FLAC3D. In the experiment, the upper and lower boundaries are simultaneously moved at a rate of 5×10^{-7} m/s (Figure 5), and the FISH language is used to monitor the stress and strain parameters in the model. Take Mohr-Coulomb model as the material constitutive model, and the physical and mechanical parameters of the material are given in Table 2.

4.1. Effect of Porosity on Compressive Strength. For the porosity of 0%, 1.86%, 3.7%, 7.4%, and 11.2%, a total of models were subjected to uniaxial numerical tests. The stress-strain curve of model with porosity 0% is shown in Figure 6. According to the stress-strain curves of different models, the variation of compressive strength with porosity is obtained (Figure 7).

From test result analysis, with the increase of porosity, the compressive strength of different pore model decreases and porosity and compressive strength shows negative exponent relationship. The model with porosity of 11.2% has the minimum compressive strength of 31 Mpa, which is 8.58% lower than the maximum compressive strength 33.91 Mpa of the model with porosity of 0%. Because the pore size distributions of different porosity models in the experiment have the same exponential distribution, the number of pores and the distribution of pores have the greatest influence on the compressive strength of the model. With the increase of porosity in the model, the damage of the model increases and the compressive strength decreases.

The experimental results show that there is a nonlinear relationship between porosity and compressive strength.

TABLE 2: The physical and mechanical parameters of materials in the model.

Density ρ (Kg/m ³)	Elastic modulus E (GPa)	Poisson's ratio ν	Cohesion c (MPa)	Angle of internal friction φ (°)	Tensile strength σ (MPa)
1261	2.3	0.35	1.9	40	1.37

FIGURE 4: Three-dimensional cylinder pore models for different porosities with 1.86%, 3.7%, 7.4%, and 11.2%.

4.2. Mechanical Properties of Different Porosity Models. Stress slice of the cylinder model has a porosity of 0%~11.2% at its height of 50 mm (Figure 8).

The experimental results show that the stress distribution of different porosity models is obviously different. The stress distribution of the porosity model with porosity 0% is symmetrical, and the stress distribution becomes more inhomogeneous with the increase of porosity.

The plastic zone of different models at the peak value of stress-strain curve shows that the failure zone is in the plastic

deformation stage (Figure 9). According to the stress-strain curve of the rock under uniaxial compression, the cylinder is in the stage of unstable fracture development, and the rupture of this stage is developing until the specimen is completely destroyed. The results show that the failure zone is in the plastic deformation stage.

In this paper, the uniaxial compression of the cylinder model with different porosities was carried out in the same loading rate and time step, and the plastic zone of the failure process of each model was obtained (Figure 10).

FIGURE 5: Schematic diagram of uniaxial loading.

FIGURE 6: The stress-strain curves of nonporosity model.

The results of numerical simulation are analyzed as follows:

- (1) At the porosity of 0% damage shows symmetric form. In the initial state of model loading symmetrical shear crack appears at the upper and lower ends of the model. With the increase of loading steps, X shaped crack extends gradually to the middle position of the specimen. At the peak of loading the cylinder rupture and the cracks at the upper and lower ends convergent in the middle, cylindrical damage is mainly shear failure.
- (2) The destruction of the model with porosity 1.86%~3.7% basically shows symmetric form; at the initial loading stage, crack shear failure model is irregular. With the increase of the number of steps of loading, crack failure gradually extends to the middle position; the crack failure is X shape, influenced by some of the cracks in the pores of slight deformation; when the model is destroyed, cracks at both ends

FIGURE 7: The relationship between compressive strength and porosity.

converge to the middle and extend to both sides, and the failure mode is mainly shear failure.

- (3) The destruction of the model with porosity 7.4%~11.2% shows asymmetrical form; at the initial loading complex failure cracks appear. With the increase of loading steps, destruction crack expands rapidly; crack of the right and left sides gradually merged and extended to the middle position; at the upper end and the lower end "V" shaped failure formed. When the model is damaged, the cracks at the two ends converge in the middle and extend to both sides, with damage in the form of shear failure.
- (4) For different models, the X shaped conjugate slant shear damage is the most common; that is, the angle between the normal vector of damage and the axis of specimen surface is 60 degrees.

FIGURE 8: The stress distributions with different porosities with 0%, 1.86%, 3.7%, 7.4%, and 11.2%.

FIGURE 9: Plastic zone of peak stress and strain of different porosity models.

Based on the analysis of shear strain increment cloud diagram of different porosity models, the expansion trend of the failure surface is obtained (Figure 11). The shear strain area of different porosity model meets the breaking angle law of $45^\circ + \varphi/2$. The shear strain of the model with 0% porosity is symmetrical, with increasing porosity of shear strain area having the characteristics of uneven distribution; the main reason is the uneven stress distribution caused by the different pore diameter and distribution in the cylinder.

- (1) When the porosity is smaller, the distribution of the pore has less cumulative effect.
- (2) When the porosity is larger, the increase of the pore number and the pore size have a significantly increasing effect on the cumulative effect of the stress.

5. Numerical Simulation of Seepage Flow in Pore Reconstruction Model

Seepage numerical simulation was taken on a 3D pore reconstruction model with porosity of 7.4%. In the loading process, certain axial pressure P_1 , lateral pressure P_2 , and pore pressures P_3 , P_4 were added initially; then displacement control loading was used in the whole loading process, with

loading displacement increment $\Delta s = 0.01 \text{ mm}$, $P_2 = 4 \text{ MPa}$, $P_3 = 2.3 \text{ MPa}$, and $P_4 = 3.8 \text{ MPa}$.

- (1) The evolution law of the coal sample loading step-vertical load-permeability coefficient is described; the consistency between the change of permeability coefficient and the crack growth is verified (Figure 12). At the same time, the initiation and propagation of crack play a very important role in the selection of flow paths.
- (2) Compared with the pore water-free pressure test, the pore water pressure test specimen is easier to produce micro crack and to be destroyed, and the failure surface is more complex, the peak value of vertical load is also reduced by 3%, and the number of steps is also two steps ahead (Figure 13).
- (3) When the models have the same porosity, their permeability variations changed considerably, which indicates that the pore structure characteristics have important influence on the permeability of the model.

6. Conclusions

- (1) Based on SEM test, we have obtained the pore structure parameters of low permeability coal seam

FIGURE 10: The failure process of different porosity models.

by MCMC and digital image processing methods. And on this basis, three-dimensional cylindrical pore models with different porosity (1.86%, 3.7%, 7.4%, and 11.2%) have been constructed.

(2) Uniaxial compression tests of different pore models reveal the influence of pore structure parameters on the physical and mechanical properties of coal and rock mass:

① porosity and compressive strength curve have negatively exponential relationship, and the quantity and distribution of pore have the greatest influence on the compressive strength of the model;

② under different porosity, the stress distribution is different. With the increase of porosity, the stress distribution gradually becomes nonuniform;

③ the compressive failures of different pore models are mainly shear failures, and the shape of fracture section is related to porosity;

④ the pore structure parameters have different influence on the stress concentration of the model. When the porosity is smaller, the distribution of the pore has less cumulative effect; when the porosity is larger, the increase of the pore number and the pore size have an obvious increasing influence on the cumulative effect of the stress.

FIGURE 11: The shear strain increment with porosities of 0%, 3.7%, and 7.4% (from left to right).

FIGURE 12: Numerical simulation results of the load step-vertical load-permeability coefficient.

FIGURE 13: Comparison of step number and vertical load curve with pore water pressure and no pore water pressure.

- (3) The evolution law of the coal sample loading step-vertical load-permeability coefficient is described. The consistency of the crack growth and the variation of the permeability coefficient are verified. At the same time, the influential mechanism of the pore structure parameters on the permeability coefficient of coal and rock is revealed.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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