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A Study on the Structure of Rock Engineering Coatings Based on Complex Network Theory

Dayu Ye [1,2], Guannan Liu [1,2,3,*], Feng Gao [1,2], Xinmin Zhu [1,2] and Yuhao Hu [1,2]

1 State Key Laboratory for Geomechanics and Deep Underground Engineering, China University of Mining and Technology, Xuzhou 221116, China; theoye@cumt.edu.cn (D.Y.); fgao@cumt.edu.cn (F.G.); TS18030215P31@cumt.edu.cn (X.Z.); TS20030008A31@cumt.edu.cn (Y.H.)
2 Mechanics and Civil Engineering Institute, China University of Mining and Technology, Xuzhou 221116, China
3 Laboratory of Mine Cooling and Coal-heat Integrated Exploitation, China University of Mining and Technology, Xuzhou 221116, China
* Correspondence: guannanliu@cumt.edu.cn

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Abstract: As one of the most basic materials of engineering coatings, rock has complex structural characteristics in its medium space. However, it is still difficult to quantitatively characterize the microstructure of rock coatings, such as connectivity and aggregation degree. For this paper, based on a CT-scan model of rock coating, we extracted the network topology of a rock coating sample and verified that its microstructure parameter distribution accords with Barabasi and Albert (BA) scale-free theory. Based on this result, relying on the BA scale-free theory, a dual-porosity network model of rock coating was constructed. We extracted the network structure of the model to verify it, and analyzed the distribution of the microstructure parameters of the model, such as degree distribution, average path length and throat length distribution. At the same time, we analyzed the evolution trend of the permeability of the coating model with the microscopic parameters. Then we discuss the influence of the change of structural parameters on the microstructure of the coating model, and compared with the mainstream rock models at the present stage, the rationality and accuracy of the models are analyzed. This provides a new method for studying the mechanical and permeability properties of engineering coating materials.

Keywords: structure of engineering coatings; pore network model; complex network theory; geometric distribution

1. Introduction

Engineering coating refers to the deposition or combination of functional materials on the surface of basic solid materials. The properties and effectiveness of engineering coatings are higher than that of basic solid materials. As coatings, rock materials are widely used in engineering. For example, in order to prevent the deformation or collapse of surroundings, the supporting lining is built with rock and other materials around the tunnel body. In many cases, the structural characteristics are the key factors affecting the mechanical and physicochemical properties of coatings [1,2]. Therefore, it is of great significance to analyze the structural characteristics of natural rocks to improve the mechanical properties of rock coatings [3]. As the mainstream research method of rock microstructure, the pore network model has been widely used. The structure of rock coating can be regarded as a pore network model, and the microstructure of rock is characterized by a pore structure connected by throats. However, rock formation is dense and the pore shape is complex, so it is still difficult to accurately characterize the rock structure and describe the pore connection mode in the pore network models [4].

In recent decades, a great deal of research has been carried out on the microstructure and physical properties of rock mass [5–9], and different kinds of rock numerical models have been established. However, due to the complexity of pore distribution in macrostructure (i.e., geometric structure of network) and micro-structure (i.e., the connection between single pore and other pores), it is still challenging to accurately describe the microstructure of rock coatings.

A key difficulty is that the throats connecting pores are often irregular and unevenly distributed, and the structural characteristics are not uniformly distributed. At present, the characterization of the rock structure mainly adopts the Bieuler number, or macroaverage perspective, which is based on the regular network. Experimental results show that rock pore structure is highly complex, and regular network models and current mainstream real-rock topology models still have great difficulties in characterizing pore connectivity and other topological structures [10–12].

With the advent of the small world model [13] and scale-free model [14], the theoretical framework of modern complex networks was initially formed. In the past 10 years, as a new interdisciplinary field, complex network theory has penetrated into many disciplines from life sciences to physics [15,16]. In previous studies, we found that the porosity degree distribution in the pore structure network of rocks shows the trend of power-law distribution, where the degree of a pore is the number of the pore connected with other pores. That is, with the increase of the number of connected other pores, the number of the pore tends to decrease in power-law ratio. And in the pore network structure of rock, those pores which connect with more other pores play a more important role [17]. Therefore, the scale-free network, that is, the connection network with power-law characteristics of pore degree distribution, can reasonably describe the topological structure of a rock coating network.

The following are several pore network research models that are used to characterize the geometric structure and microscopic characteristics of rocks. The purpose of the model and the research results are summarized in Table 1.

Table 1. Research models used to characterize the microscopic characteristics of rocks.

Author	Years	Purpose of Model	Research Result
Blunt et al. [11].	2002	Research on microscopic effective transport properties based on coordination number rules	A network model that uses additional coordination numbers and is simulated as having irregular connectivity is established.
Hou et al. [18].	2006	Establish a microstructure model considering pore throat radius and shape factor	Figured out that the pore throat radius and shape factor were the main factors affecting polymer retention.
Wang et al. [19].	2007	Explore the influence of reservoir pore structure parameters on water saturation	A network model which can reflect the pore structure of a reservoir is established.
Yao and Tao [20]	2007	Build 3D cubic network model	A mathematical model for solving capillary pressure and relative permeability is established.
Ghous [21]	2008	Explore the influence of pore structure characteristics on rock resistivity	The effects of the structural characteristics of macropores and micropores on rock resistivity at different scales are obtained.
Wang et al. [22].	2013	Establish a multiscale pore network model	Based on the three-dimensional regular network model, a carbonate multiscale network model is constructed.

Based on the porous media [23] and the rock mass digital model [24,25], the Barabasi and Albert (BA) scale-free connection method is used to establish a dual-porosity network model of rock. The porosity degree distribution, average path length, throat length distribution and other parameters of the rock model are used to quantitatively describe the connection of rock pores and throats. The evolution trend of the permeability of the coating model with the microscopic parameters was analyzed. This provides a theoretical basis for the analysis of mechanical properties and physicochemical properties of rock, offering technical support for the more reasonable development and utilization of rock coatings.

2. Characteristics of Rock Pore Network Structure

In this section, we first introduce the research method of rock coating pore network and the mainstream pore network model at the present stage. We made four kinds of rock samples with

different porosity and analyzed the microscopic parameters [17]. It is verified that the microstructure of the coated rock accords with the BA scale-free connection mode, as shown in Figure 1.

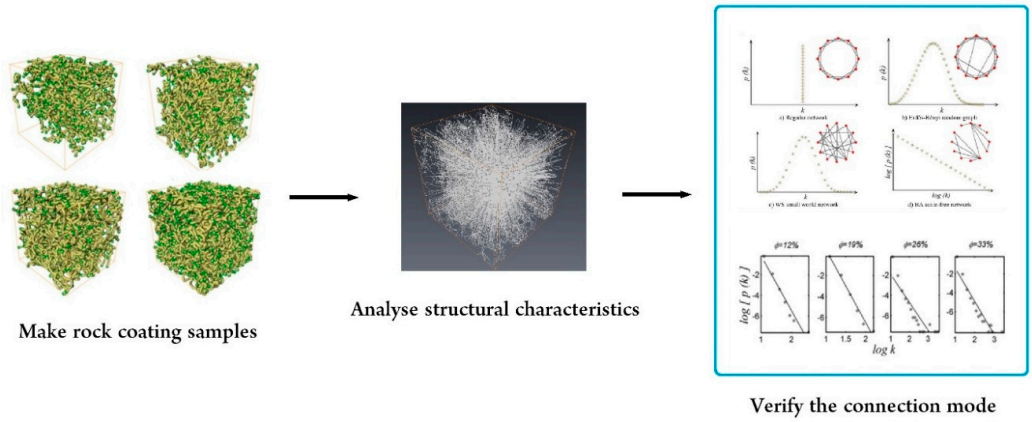

Figure 1. Verification of pore structure of rock coating.

In recent years, as an emerging interdisciplinary field, complex network theory has gradually penetrated into biology, sociology and many other disciplines [26]. Regular network, ER (Erdős–Rényi) random network and WS (Watts-Strogatz) small world network are three classic models describing the structure of random networks. The structure of rock can be regarded as a pore network model, and its microstructure is the pores connected by the throats. As shown in Figure 2.

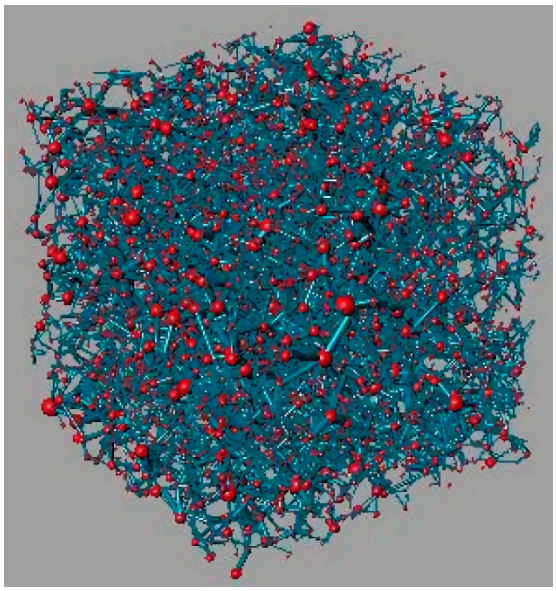

Figure 2. Pore network structure of rock coating.

Regular network, as shown in Figure 3a, the network degree k (the number of edges connected to the node) is the same value, and the regular network has the smallest average path length in all networks with the same number of nodes (the average of all nodes short distance) $L = 1$, $P(k)$ represents the probability of the node. In ER random network, as shown in Figure 3b, the connection probability of two nodes is P, regardless of whether they have a common neighbor node. The degree of most nodes is k, the degree distribution conforms to the Poisson distribution, and the average path length is relatively high.

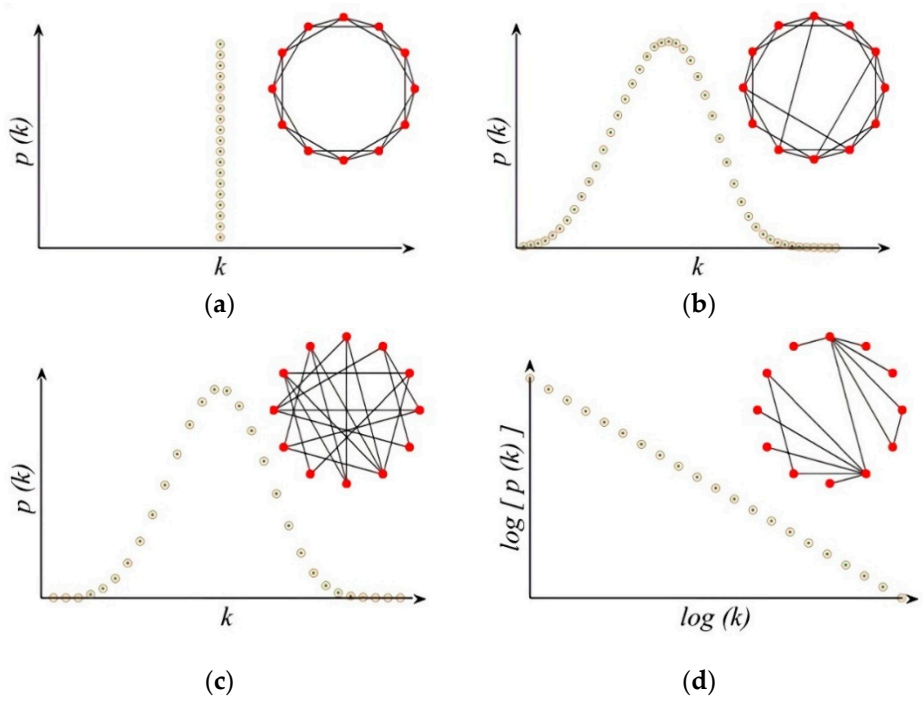

Figure 3. Different network model structures. (**a**) Regular network; (**b**) Erdős–Rényi random graph; (**c**) Watts-Strogatz small world network; (**d**) Barabasi-Albert scale-free network.

As a transition from a regular network to a random network, Figure 3c shows the degree distribution of the WS small world network. Most nodes are not connected, but different nodes can be reached by fewer edges.

Empirical research shows that other real networks such as the mobile internet and cellular metabolic networks are irregular networks, and the connectivity distribution function takes the form of a power rate [27]. In order to explain the generation mechanism of the power-law distribution, Barabasi and Albert proposed a scale-free network model, namely the BA scale-free model [14]. As a model for describing heterogeneous networks, the degree distribution function of the BA scale-free network is:

$$P(k) = \frac{2m(m+1)}{k(k+1)(k+2)} \propto 2m^2k^{-3} \quad (1)$$

where m is the number of new nodes connected to existing nodes during network expansion, namely:

$$P(k) \approx k^{-\gamma} \quad (2)$$

Among them, γ is power exponent, and there is no obvious characteristic value (Figure 3d), but it is extremely robust to random node failures. As long as the few nodes with the largest degree in the network are consciously removed, it will have a huge impact on the connectivity of the entire network.

In the previous research [17], we used the pressing method to produce artificial sandstone with porosities of 12%, 19%, 26% and 33% through different ratios of 50–300 mesh natural sandstone powder and epoxy resin. An X-ray synchrotron radiation imaging experimental device with an effective pixel resolution of 12–14 μm is used to scan and generate a tomographic image stack. Then, the pore network model is established by using the ossification algorithm to take the pore as the node and the throat as the edge to extract the pore structure information. As shown in Figure 4. At the same time, in order to study the microstructure of different structural rocks, we analyze the characteristics of the rock network with different porosity.

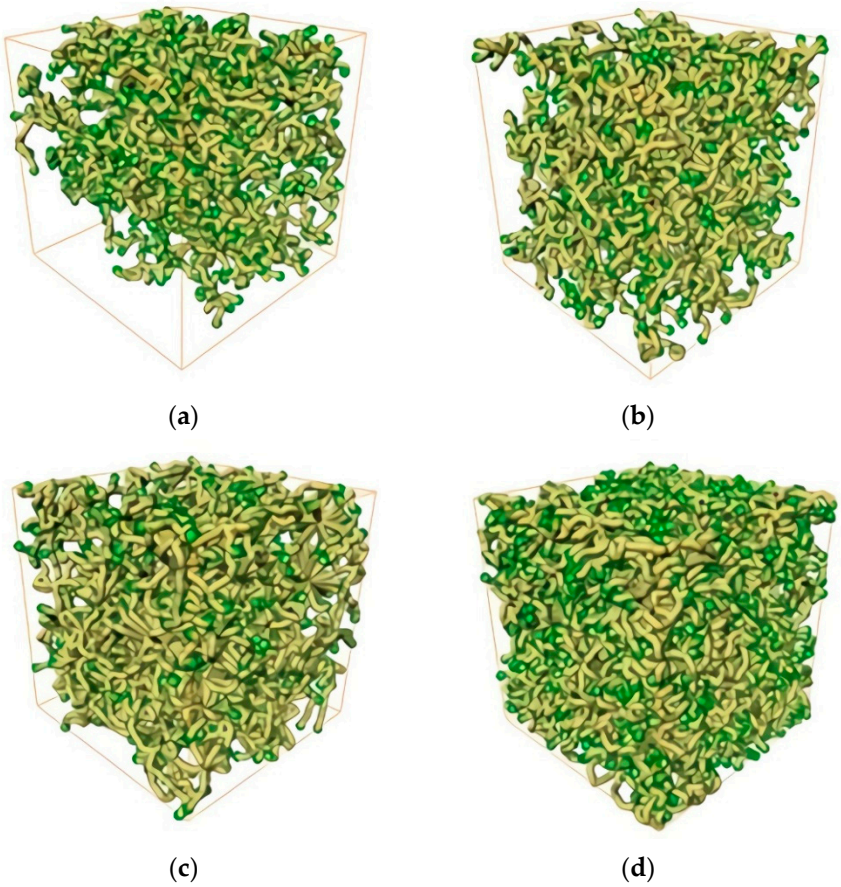

Figure 4. Three-dimensional sandstone pore network. (**a**) porosity = 12%; (**b**) porosity = 19%; (**c**) porosity = 26%; (**d**) porosity = 33%.

The distribution function $P(k)$ is used to represent the distribution of network node degrees. $P(k)$ represents the probability that the randomly selected node degree is k. In the rock coating network model, the degree of a pore is the number of the pore connected with other pores. The experimental results show that the pore network of different degrees satisfies the power-law distribution, as shown in Figure 5. Therefore, the rock network conforms to the BA scale-free network, that is, there are a small number of scale-free network height nodes called the "hub" of the network. In a sense, these joints may play a leading role in the deformation and failure process of rock under load and stress distribution [28,29].

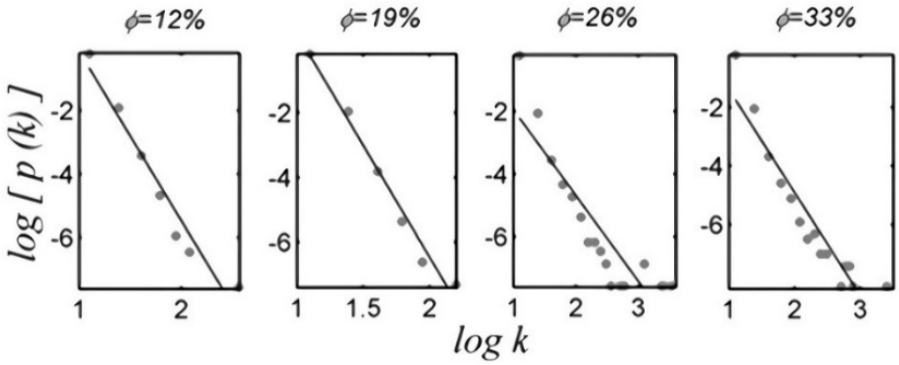

Figure 5. Distribution curve of degree k of sandstone structure.

3. Construction of Three-Dimensional Rock Pore Network Model Based on BA Scale-Free Connection

The construction of the pore network model retains the properties of the real macropore network model and the micropore network model as much as possible, and the geometric topology of the pore network model is an important evaluation criterion to ensure the accuracy of the model. Wang proposed a theoretical method to integrate and construct a dual-porosity network model [30]. First, determine the spatial domain Ω of the large-pore network reconstruction, that is, determine the geometric size of the dual-porosity network model. Based on a real-rock model size, it is assumed that the number of pores is N_p, the network volume is $V = lwh$ and $l = w = h$. The number of macropores in the established pore network is N_p', the network volume is $V' = LWH$ and $L = W = H$. Therefore, the size factor is:

$$\xi = L/l = W/w = H/h \tag{3}$$

Then we can obtain:

$$N_p' = \xi^3 N_p \tag{4}$$

We introduce the BA scale-free connection method in the complex network theory to generate and connect the nodes in the pore domain. BA scale-free network meets the following two characteristics:

- Growth: Starting from a network with m_0 nodes, each time a new node is introduced and connected to m existing nodes, where $m \leq m_0$.
- Optimal connection: The probability $\prod_i$ of a new node j connected to an existing node i, the degree k_i of node i, and the degree k_j of node j satisfy the following relationship:

$$\prod_i = \frac{k_i}{\sum\limits_j k_j} \tag{5}$$

After t steps, the algorithm will generate a network with $N = t + m_0$ nodes and mt edges, that is, the program will generate a pore network model with N pores and mt throats. Changing the parameters of m_0 and m in the BA scale-free network will change the structure of the pore network model accordingly.

At the same time, the average path length of the BA scale-free network structure, that is, the average length of the throats, has the following relationship:

$$L = \frac{1}{\frac{1}{2}N(N+1)} \sum_{i \geq j} d_{ij} \tag{6}$$

where d represents the shortest path length between any two nodes (the minimum number of edges connecting any two nodes), and N is the total number of network pores.

During the process from m_0 to N_p', the generated pore cannot coincide or overlap with the existing pore. That is, when a new pore k with a radius of r_k is generated, it should satisfy that it will not cover the generated pore $j(j = 1, 2, ..., k-1)$, that is:

$$r_k + r_j < d_{jk} \tag{7}$$

where d_{jk} is the Euclidean distance between pores k and j. It is only necessary to determine the radius of the new pore and the pore radius which has been generated in the adjacent small area around it.

According to the distribution of the pore radius of the real-rock model, we determined the value range of the large pore radius in the dual-porosity model. And randomly generate large pores with a radius within the value range at the pore center coordinate point of the large pore space domain.

So far, the macropore network model based on the BA scale-free network has been established. The filling of the micropore network refers to the generation of micropores and microthroat unit bodies based on the BA scale-free network connection method in the generated macropore network skeleton space. It mainly includes the steps of determining the spatial domain of the micropore network, generating equivalent micropores, and constructing throats between micropores.

The micropore network cannot overlap with the macropore network during the filling process, so the space domain filled by the micropore network is the skeleton space of the macropore network. Assuming that the overall space of the pore network model is Ω, the pore space of the constructed macropore network is Ω_1, and the space domain of the micropore network model to be constructed is Ω_2.Then the micropore space domain can be expressed as:

$$\Omega_2 = \Omega - \Omega_1 \tag{8}$$

Analogous to Equation (4), we can get the number of micropores to be constructed in the micropore network:

$$N_{pm}{}' = \xi^3 N_{pm} \tag{9}$$

Among them, N_{pm} is the number of micropores in the real-rock digital model.

Similarly, we use the BA scale-free connection method (Equation (5)) to generate the microporous network model. The connection method of the micro throat is similar to that of the large throat. At the same time, before a new micropore is generated, it must be ensured that it will not cover the micropores that have been generated. The judgment condition is the same as Equation (7).

However, at this time, the newly generated macropore network and the micropore network are not connected, so it is necessary to add a connecting throat between the macropore and the micropore to integrate the dual-porosity network. Wang [30] proposed a connection construction method that integrates a two-scale network model. At the center of the original micropore network, place the pore body with the smallest radius in the macropore network, and calculate the coordination number between the surface of this pore and the surrounding micropore throat. By increasing the radius of the pore body, the coordination number of a series of pore surface and the surrounding micropore throat can be obtained, and then the coordination number distribution map between the macropore and the micropore can be obtained. According to the coordination number distribution map between the macropores and the micropores, the connecting throats between the macropores and the adjacent micropores are added.

Through the above steps, the established macroporous network based on the BA scale-free connection mode can be integrated with the microporous network, and then a dual-porosity network model based on the BA scale-free network connection mode is constructed.

4. Results and Analysis

We use the Carbonatite digital model proposed by the Martin Blunt team of Imperial College London [31]. At the same time, based on the size of the real-rock model, combined with Equations (3), (4), (8) and (9), the scale factor ξ is selected. We determined the number of pores in the macropore network model (N_p') and the number of pores in the micropore network model (N_{pm}'). Combining the BA scale-free connection principle and the above equations, we constructed a dual-porosity rock coating network model. As shown in Figure 6.

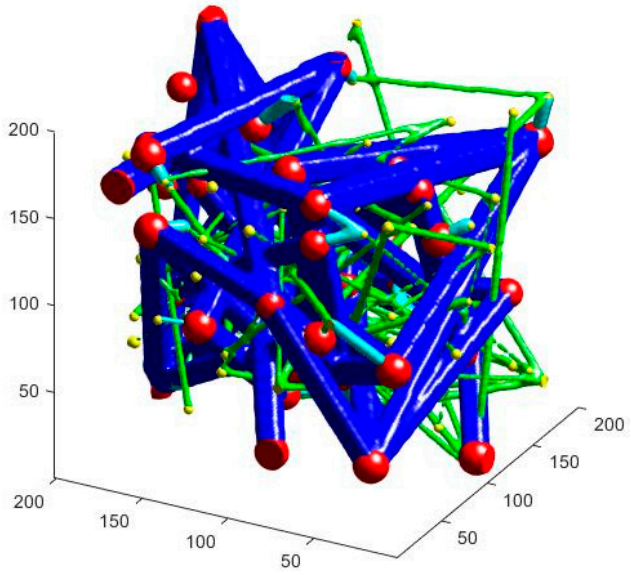

Figure 6. Two-scale network model based on BA scale-free network connection.

To verify the correctness of the model, we extracted the digital structure characteristics of the pore network of the real-rock digital model, and analyzed the degree distribution of the pore network model, as shown in Figure 7.

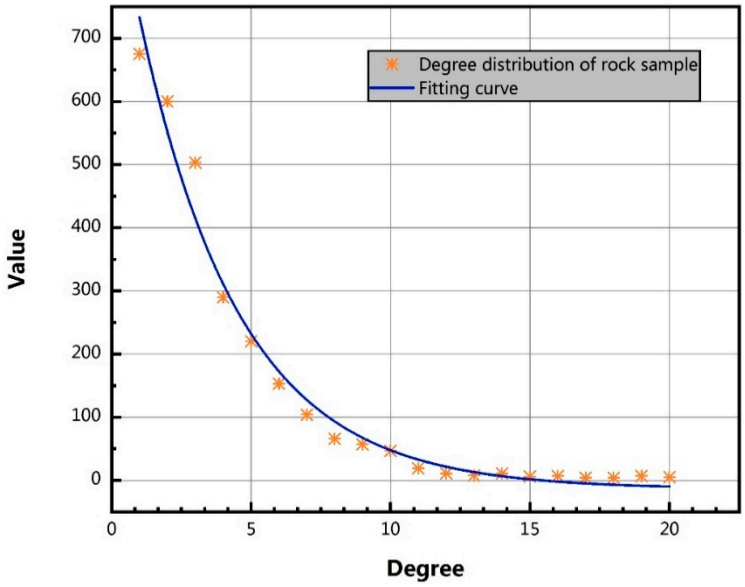

Figure 7. Distribution characteristics of the carbonate sample.

It can be seen from Figure 7 that the distribution characteristic of the real-rock pore network degree accords with the property of power ratio distribution. The characteristic of its distribution function accords with the Equations (1) and (2), that is, the BA scale-free network connection is the main connection mode of the rock pore network.

Similarly, we analyzed the structural characteristics of the dual-porosity rock coating network model based on the BA scale-free network, and analyzed its degree distribution characteristics. Using the size factor method proposed by Wang [30], the model degree distribution value is multiplied by the size factor obtained above, and the revised model degree distribution trend is obtained. The revised model degree distribution characteristics and real-rock degree distribution characteristics are shown in Figure 8.

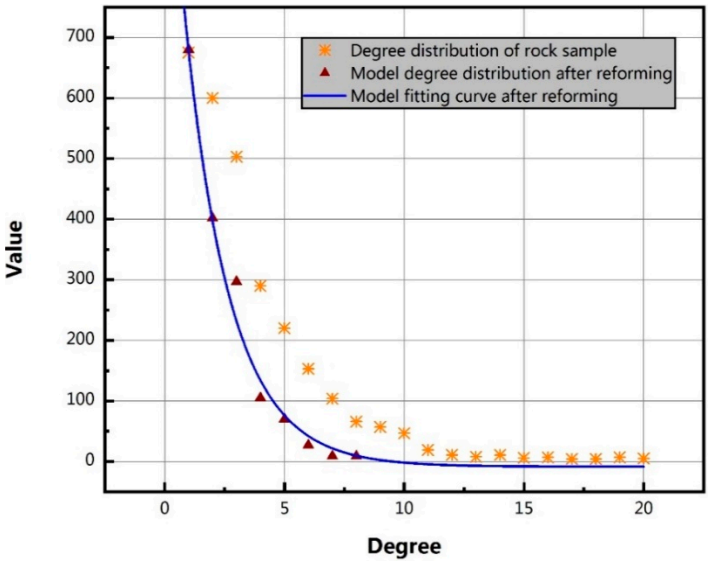

Figure 8. Comparison of the revised model and real-rock degree distribution characteristics.

It can be seen from Figure 8 that the degree distribution characteristics of the dual-porosity network model proposed in this paper are in good agreement with those of the real-rock sample. In order to further verify the correctness of the model proposed in this paper, we selected four different rock samples. By extracting the network structure and parameter analysis of them, we have obtained the degree distribution characteristics. At the same time, by changing the specific parameters m_0 and m in the BA scale-free network (Equation (5)), we established four different dual-porosity network models and analyzed the structural characteristics of the network models. The degree distribution characteristics of the four different network models and the rock samples are shown in Figure 9.

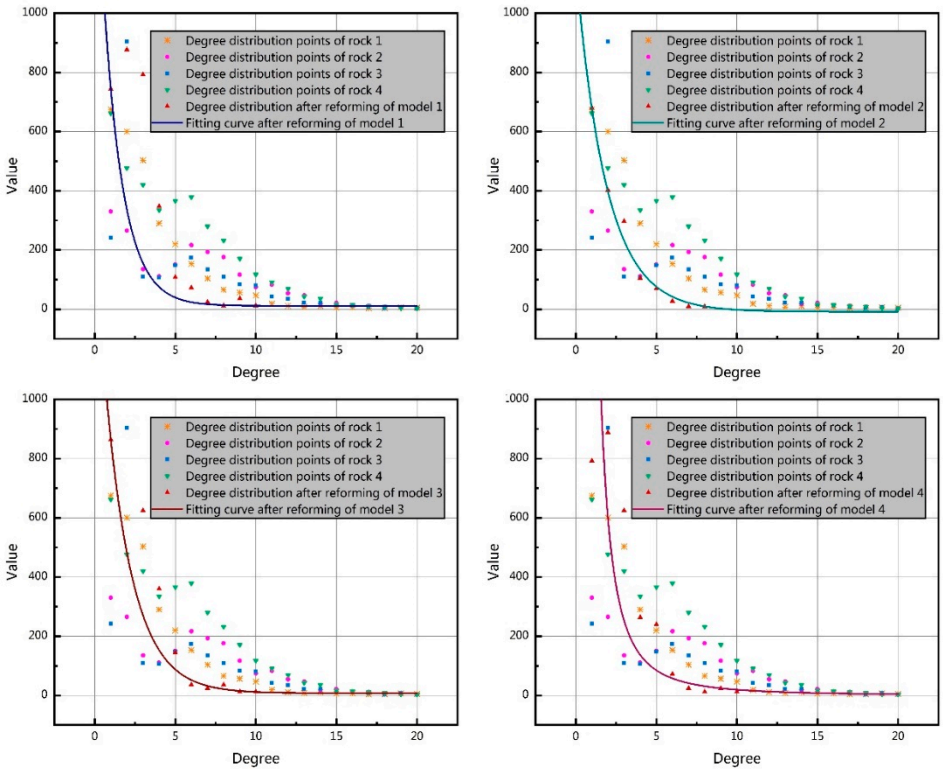

Figure 9. Comparison of distribution of four different rocks with different models.

From Figure 9, we can see that although the fitting curve of the model changes with the change of m_0 and m, it is still in good agreement with the degree distribution characteristics of the rock samples. That is, the model proposed in this paper can well describe the structural characteristics of the rock coating pore network.

Meanwhile, we explored the effects of different degree distributions on network permeability. We analyzed the degree distribution of four different rocks and calculated the network permeability of these four rocks, as shown in Figures 10 and 11.

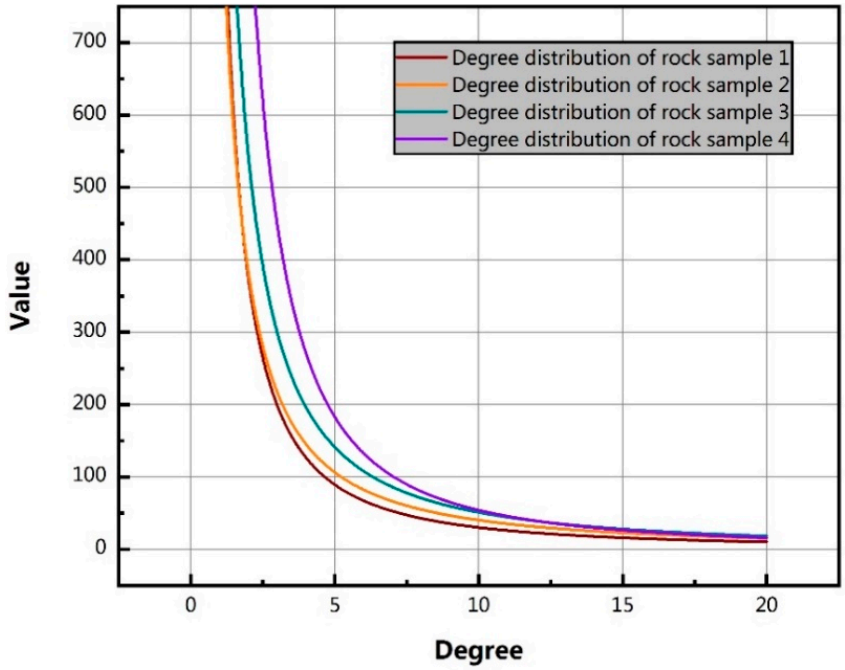

Figure 10. Degree distribution of four different rocks.

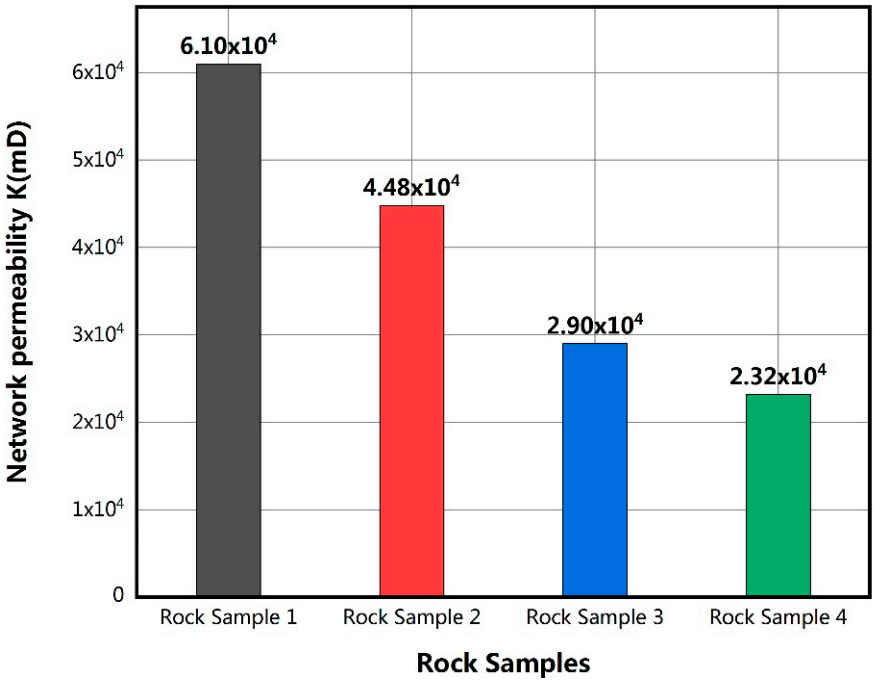

Figure 11. Network permeability of different samples.

From Figures 10 and 11 we can see that the permeability of the rock network model is closely related to its degree distribution. With the increase of the number of pores with small degree in the rock network model, the overall permeability decreases. If the degree of a pore is small, the number of throats connected by this pore is small, and the number of pores connecting other pores is also small. In the process of rock seepage, with the increase of the number of pores with weak connectivity, the seepage intensity decreases and the permeability also decreases.

Then, we analyzed the influence of m_0 and m on the rock structure. First of all, we analyzed the influence of structural parameters on the degree distribution of the network model. Since macropores play a leading role in the process of load and stress distribution of rock, in order to simplify the calculation, we constructed a two-dimensional large pore network model equivalent to the real-rock size. After that, we changed the value of m_0 and m, analyzed the degree distribution of each model, and compared it with the degree distribution of rock samples. The degree distributions of the models under different m_0, m and the degree distribution of the rock sample are shown in Figure 12.

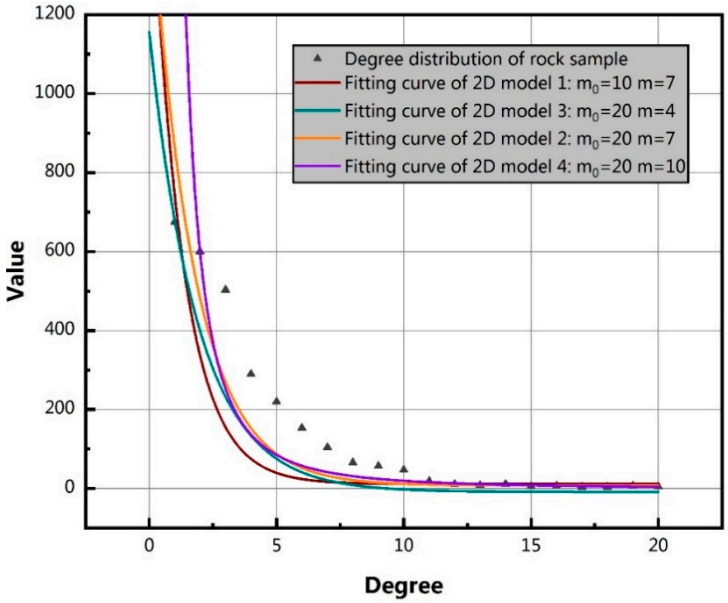

Figure 12. The characteristics of degree distributions under different m_0 and m.

From Figure 12, it can be seen that the degree distributions under different m_0 and m strictly obey the power-law distribution, and are in good agreement with the distribution characteristics of the rock sample degree. When m and other microstructure parameters remain unchanged, the number of the pores with the degree between two and seven increases with the increase of m_0. When other parameters remain unchanged, with the increase of m_0, the number of pores with degrees one and two increases sharply. And the number of pores with a higher degree value does not change much with the change of m_0 and m.

The average path length of the rock coating model, that is, the average length of the throat connecting the rock pores in the pore network, plays an important role in analyzing the stress distribution and failure characteristics of the model. When other parameters such as rock porosity, size and structure remain unchanged, based on Equation (6). We analyzed the evolution of the average path length of the model under different values of m_0 and m, as shown in Figure 13.

From Figure 13, we can conclude that the average path length of the model increases with the increase of m_0 and m, when other parameters are identical. And m has a greater impact on the average path length. With the increase of the average path length, there are more throats in the network. This will lead to the uneven stress distribution of rock under loading, which is more likely to cause the

failure of rock coating. Therefore, we speculate that from the perspective of the average path length, the increase of m_0 and m is not conducive to the stress process of the rock coating.

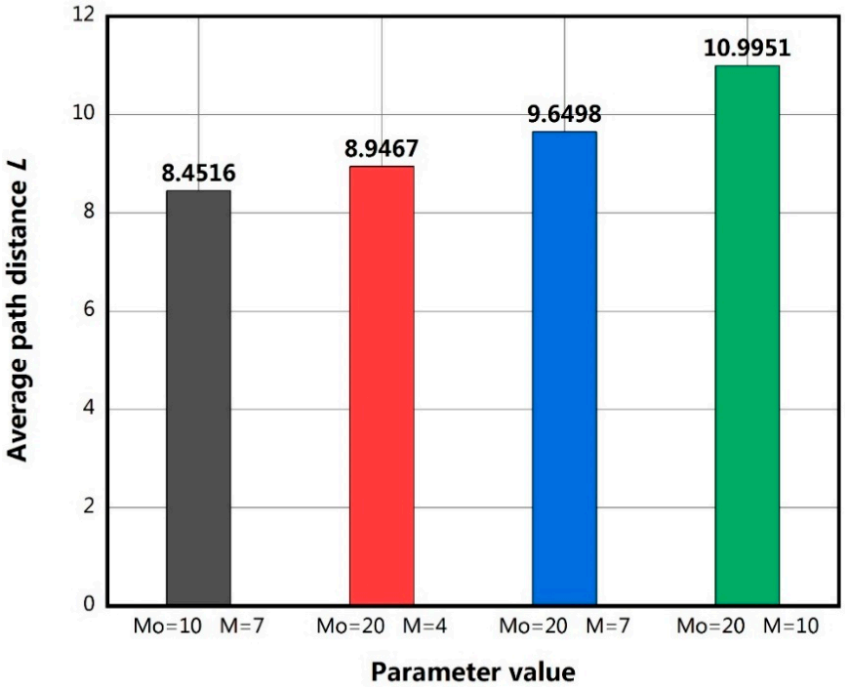

Figure 13. Evolution of the average path length under different values of m_0 and m.

In order to further explore the influence of the value of m_0 and m on the coating, we explored the distribution of rock throat length. We selected the above-mentioned Carbonatite digital model proposed by Martin Blunt's team [31] based on CT tomography, extracted the network structure and analyzed its throat distribution, as shown in Figure 14.

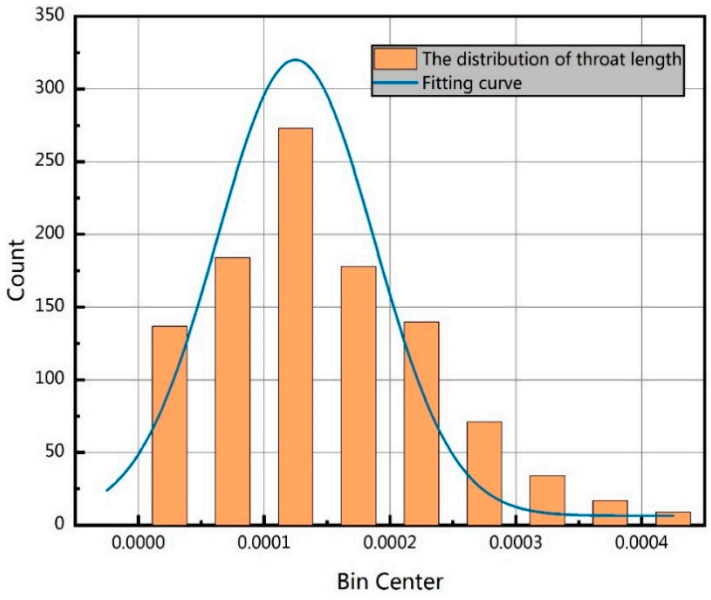

Figure 14. The throat length distribution characteristics of carbonate samples.

From Figure 14, we can conclude that the distribution of rock throat length roughly presents a Gaussian distribution. The length of the throats is mostly concentrated in the range of (0.00005–0.00015), and the number of throats with larger length is much smaller than that of those with smaller length.

Similarly, we changed the values of m_0 and m, and analyzed the throat length distribution of each model, as shown in Figure 15. The network parameters such as the size and the number of pores of each model are the same as those of the rock samples.

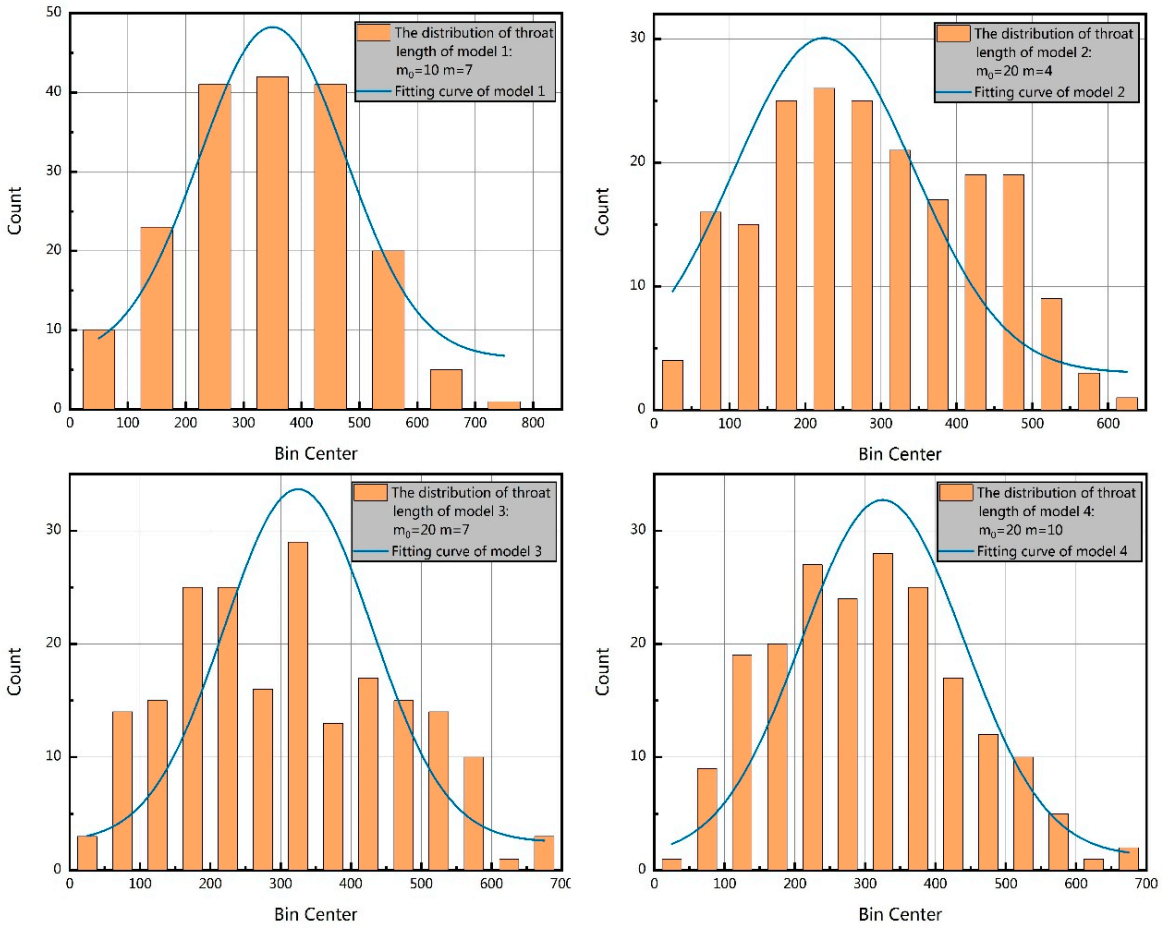

Figure 15. The distribution characteristics of throat length under different values of m_0 and m.

Figure 15 shows the effect of m_0 and m on the throat length distribution of the rock coating. The throat length distribution characteristics of the four models are consistent with the distribution of the rock sample. When the value of m_0 is 10, the throat length is mainly concentrated in the range of 250–550, and there are throats of larger length (greater than 700). With the increase of m_0, the length of the throats is mainly distributed in the range of 75–450. That is, as m_0 increases, the throat length generally shows a decreasing trend. At $m = 4$, the length of throats is small (75–350), as m increases, the concentrated interval of throats length also increases. That is, with the increase of m, the overall throat length shows an increasing distribution trend.

Then, we analyzed the degree distribution of different rock network methods in the current mainstream models. The ER random network, WS small world network and conventional regular rock connection models were selected.

Where the degree distribution of the ER random graph satisfies [32]:

$$P(k) = \begin{pmatrix} N-1 \\ K \end{pmatrix} P^k (1-P)^{N-1-k} \approx \frac{\langle k \rangle^k}{k!} e^{-\langle k \rangle} \tag{10}$$

where *P (k)* is the probability that the degree of a pore is k, and N is the total number of pores in the network. The construction algorithm of WS small world model is as follows [13]:

(1) Start modeling with a ring of regular networks: The network contains N nodes, and each node connects to the K nodes closest to it. Where $N >> K >> ln(N) >> 1$.

(2) Randomize reconnection: reconnect each edge in the network randomly with probability p, that is, one endpoint of the edge remains unchanged, while the other endpoint is taken as a randomly selected node in the network. It stipulates that there can be at most one edge between any two different nodes, and each node cannot have an edge connected to itself.

And the total number of nodes in different networks is consistent with the number of pores in the rock samples. We compared the degree distribution of different models with that of the rock sample, as shown in Figure 16.

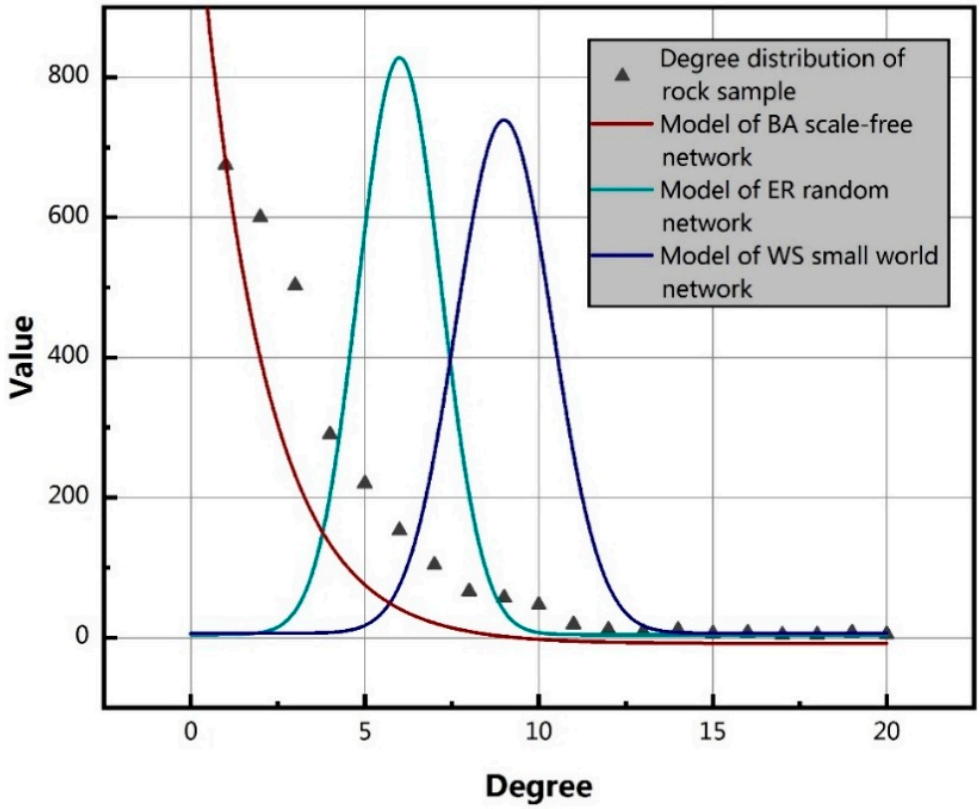

Figure 16. Comparison of different models with real-rock distribution characteristics (note: the degree distribution of regular model is the points of degree = 2, 3, 4, and 6).

From Figure 16, we can conclude that the current conventional pore network model is not in good agreement with the structural characteristics of the rock sample compared with the BA scale-free connection model, where the degree distribution characteristics of the real-rock sample is power-law distribution, and the rock coating model proposed in this paper is also power-law distribution. However, the degree distribution characteristics of the ER random network and WS small world network models are Gaussian distribution, and the regular rock connection model is point distribution, which do not match the degree distribution characteristics of the real-rock sample.

Therefore, the pore network model based on a BA scale-free connection can describe rock structure more accurately. It provides theoretical basis and technical support for the analysis of rock mechanical properties and physicochemical properties, and more reasonable development and utilization of rock coatings. At the same time, because we study the microstructure of rock coatings, the analysis of the entire coating requires a large number of samples, which may have cost-effective limitations. Although the model is not compared with the permeability results in the published study, the microstructure has been compared with the actual rock samples, which is Figures 8 and 9.

In addition, this study uses the method of compiling the numerical model of a pore network to simulate the actual coated rock, so there is no error analysis, which may cause numerical limitations. Since we only consider the characteristics of rock microstructure, in the next study, we will explore the influence of microparameters (such as degree distribution, average path length, throat length, etc.) on the mechanical and physicochemical properties of the overall coating.

5. Conclusions

The rock pore structure is an important factor of coating failure. In order to analyze the microstructure of rock coating more accurately, a dual-porosity rock structure model was established in this paper. The pore connection structure was constructed by a BA scale-free method, and the rock coating model was compared with different types of real-rock samples to verify the correctness. We discussed the influence of structural parameters on the structure and permeability of the network model. The main conclusions are as follows:

- BA scale-free method can accurately and truly describe the pore structure of coated rocks. The dual-pore network model proposed in this paper can well match the structural distribution characteristics of different types of rocks, so as to reasonably describe the structure of the coating.
- With the increase of the number of pores with a small degree in a rock network model, the overall permeability decreases. And the number of the pores with the degree between two and seven increases with the increase of m_0. With the increase of m_0, the number of pores with degree one and two increases sharply, while the number of pores with higher degree value does not change much with the change of m_0 and m. Besides, with the increase of m_0 and m, the average path length of the rock shows an increasing trend. And with the increase of m_0, the overall throat length shows a decreasing trend, while the effect of m is opposite.
- Compared with the mainstream pore network model, the BA scale-free connection method can describe rock structure more accurately. This provides a new method for studying mechanical and permeability properties of engineering coating materials.

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