STUDY ON THE EVOLUTION LAW OF PHYSICAL PROPERTIES OF SOFT COAL SEAMS UNDER DIFFERENT WATER IMMERSION TIME

by

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> Original scientific paper https://doi.org/10.2298/TSCI2106515T

Aiming at the problems of easy spalling and roof fall in the soft coal seam under the influence of strong deep mining, the 31020 working face of Pingdingshan No.12 coal mine is used as the engineering background, combined with nuclear magnetic resonance, etc. Various technical methods have carried out research on the water absorption characteristics, composition, micro-structure, and fracture morphology of coal at different immersion time. The experimental results show that the coal sample in this mining area belongs to coking coal under the bituminous coal category. The main inorganic substances are kaolinite and calcite.

Key words: coal, immersion time, micro-structure, nuclear magnetic resonance

Introduction

With the depletion of shallow coal resources, deep coal resource mining has become the norm, while soft coal seams are the type of coal seams often involved in deep mining [1-3]. After the coal seam mining enters the deep part, the environment of high ground stress, high ground temperature, and high osmotic pressure in the deep is superimposed with strong mining disturbances [4, 5], and disasters such as roof fall, water disaster, gas disaster and other safety accidents seriously threaten the safe and green mining of coal [6]. In order to ensure the safe and efficient production of soft coal seams, some mines have begun to inject water into the coal wall with shallow holes to improve coal cohesion and shear strength, relieve coal wall pressure, improve coal stability, and prevent rib spalling [7]. At present, the water injection modification mechanism of soft coal seams under the influence of engineering disturbance by the academic and engineering circles mainly stays at the macro level. However, the differences in coal mineral composition, micro-structure, density and other characteristics and physical properties will affect the macromechanics of coal mass. The characteristics have a great influence [8].

In recent years, domestic and foreign scholars have carried out a lot of work on the microscopic properties of coal, the influence of water on the mechanical properties of coal, and coal water injection technology. Gong *et al.* [9] used SEM tests to find that the horizontal, vertical, and diagonal distribution of pore throats in coal matrix are statistically similar. Xu *et al.* [10] used SEM to obtain the relationship between coal pore characteristics and metamor-

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phic degree, permeability. Xia et al. [11] used SEM technology to study the structural changes of bituminous coal during natural weathering. Pan et al. [12] observed that the coal matrix micropores were round or elliptical through FESEM. Ramandi et al. [13] used X-ray and SEM to propose a precise measurement and a new method for adjusting the aperture of fractures in digital images of fractured media. Gong et al. [14] used the threshold method to extract macroscopic cracks, and proposed a multi-scale fine description method of coal pore structure based on CT image description. Zhang et al. [15] used CT scanning and 3-D reconstruction qualitatively and quantitatively study the coal spatial fracture network of three mining methods. Pant et al. [16] used micro-CT to study the multi-scale characterization of coal transportation structure. Liu et al. [17] used FIB-SEM and micro-CT to study the development characteristics and genetic types of connected pores in coal. Zhao et al. [18] proved that the pore structure distribution characteristics can be obtained directly from the linear relationship between pore volume and signal intensity by comparing NMR and liquid nitrogen adsorption methods to measure pores, and there is a high linear consistency with the liquid nitrogen adsorption data. Zhang et al. [19] used NMR testing technology to study the structural characteristics of ten coals with different levels of metamorphism in my country. Yao et al. [20] combined NMR and CT testing techniques, and proposed a new method for fine quantitative characterization of coal pore fissure types, effective porosity, pore structure distribution, and pore fissure configuration. Cheng and Pan [21] analyzed and summarized pore volume and specific surface area data based on pore size distribution characteristics of coal structures with different structural deformation characteristics. Xu [22] found that as the water content increases, the post-peak curve gradually changes from plastic softening to plastic strengthening. Huang [23] found that in addition the main fracture surface formed by the main fracture of water pressure in the hydraulic fracturing of coal, the seepage water pressure forms a water wedge effect on the coal on both sides of the main fracture, and the fracture and bedding plane have opened and expanded. Yuan and Jiang [24] carried out a triaxial permeability test and found that within the test range, as the moisture content increases, the influence of moisture on gas pressure sensitivity becomes more pronounced. The water pressure mainly affects coal sample gas pressure sensitivity by creating cracks.

At present, many useful insights have been obtained in the related research work on the interaction of water and coal. However, there are few related studies on the evolution characteristics of the micro-structure of soft coal seams considering different water immersion time. This paper takes the soft coal seam in a certain mining area of Pingdingshan coal mine as the research object, takes different water immersion time as the starting point, integrates NMR, XRD, XRF, SEM, and other micro-test methods, and systematically explores the water and the soft coal seam from the micro-level and mechanism. It captures the evolution characteristics and microscopic mechanism of coal seam pore structure under different water immersion time, provides basic understanding of the water injection modification mechanism of soft coal seams in Pingdingshan coal mine area, provides guidance for safe and efficient mining of water injected coal seams, and provides guidance for the gas mine of Pingdingshan Coal Mine Group safe and efficient mining of soft coal seams is of great significance.

Composition analysis of soft coal seam under different water immersion time

Industrial analysis of coal samples with different immersion time

Industrial analysis of coal refers to the general term for the determination of four analysis items including coal moisture, M, ash, A, volatile, V, and fixed carbon, FC. According to the analysis results, it is possible to roughly understand the content of organic matter and calorific value in coal, so as to preliminarily judge the type of coal. The XKGF-8000 automatic

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industrial analyzer is selected for industrial analysis, which is suitable for batch detection of moisture, ash and volatile of coal, coke or other organic matter, and can automatically calculate the fixed carbon value.

The calculation method of moisture, ash and volatile is given [25]. The mass fraction M_{ad} of moisture in coal sample is given:

$$M_{ad} = \frac{m_0 + m_1 - m_2}{m_1} \times 100 \tag{1}$$

where m_0 is the mass of the empty crucible, m_1 – the weight of the coal sample, and m_2 – the mass of sample and crucible after heating.

The mass fraction A_{ad} of ash on air dry basis:

$$A_{ad} = \frac{m_3 - m_0}{m_1} \times 100 \tag{2}$$

where m_3 is the mass of residue and crucible after burning.

The mass fraction V_{ad} of volatile on air dry basis:

$$V_{ad} = \frac{m_0 + m_1 - m_4}{m_1} \times 100 - M_{ad}$$
(3)

where m_4 is the mass of residue and crucible after heating.

The results of industrial analysis and testing of coal samples with different immersion time are shown in tab. 1 and fig. 1.

Immersion time	Moisture [%]	Volatile [%]			Ash [%]		Fixed carbon [%]	
		Air dry basis	Dry basis	Dry ashfree basis	Air dry basis	Dry basis	Air dry basis	Dry basis
0 hour	0.89	19.13	19.30	22.27	13.11	13.23	66.87	67.47
3 hours	0.88	19.36	19.53	22.28	12.09	12.20	67.67	68.27
6 hours	1.02	18.77	18.97	21.22	10.42	10.52	69.79	70.51
12 hours	0.94	19.40	19.59	22.08	11.09	11.20	68.57	69.22
1 day	1.20	18.63	18.86	20.53	7.95	8.05	72.22	73.10
36 hours	0.99	18.78	18.97	21.64	12.11	12.23	68.12	68.80
2 days	1.07	19.67	19.89	22.45	11.17	11.30	68.09	68.83
10 days	1.09	18.82	19.02	21.09	9.57	9.67	70.52	71.30
20 days	1.79	18.01	18.34	21.07	12.48	12.71	67.72	68.95
1 month	1.03	18.79	18.99	21.07	9.70	9.80	70.48	71.21
3 months	0.75	20.27	20.42	24.60	16.73	16.86	62.25	62.72

Table 1. Coal sample industrial analysis test result table

In general, the moisture and volatile content of coal samples at different immersion time are not much different. Based on air drying basis, the moisture content is between 0.75% and 1.2%, with an average content of 1.06% and the volatile content is between 18.86% and 20.42%. The average content is 19.06%. However, the fixed carbon and ash content are greatly affected by the immersion time. The fixed carbon and ash in the early stage fluctuate. Combined with the SEM, it is inferred that the flaky structure periodically peels off.

The volatile content of the dry ash-free base of the coal samples at each immersion time is between 20.53% and 24.60%, with an average content of 21.84%, belonging to cok-



coal samples with different immersion time

ing coal under the bituminous coal category. The dry ash-free volatile and fixed carbon content of coal are the main parameters that characterize the degree of coalification of the coal sample. The higher the dry ash-free volatile content, the lower the degree of coalification of the corresponding coal sample. The fixed carbon is the opposite, it is an important source of the calorific value of coal, which increases with the increase in the degree of deterioration. The volatile content of the dry ash-free base of the coal sample did not change significantly with the increase of

the immersion time, but the fixed carbon content of the air dry basis decreased with the increase of immersion time, indicating calorific value of the coal sample decreases with the increase of water immersion time.

Therefore, the coal sample in Pingdingshan coal mine belongs to the coking coal, but its degree of coalification and calorific value all show certain differences. The specific manifestation is that with the increase of water immersion time, the coalification degree and calorific value of coal samples show a decreasing trend as a whole, and the moisture content is basically unchanged. These differences will cause different mechanical properties of coal to some extent.

Elemental analysis of coal samples with different immersion time

The elemental analysis of coal samples with different immersion time adopts X-ray fluorescence (XRF) test method. Preparation before the test:

- coal sample soaking,
- coal sample drying,
- coal sample grinding, and
- culverized coal heating.

Through XRF spectroscopy analysis, it is obtained that the coal in the Pingdingshan coal mine area mainly contains six elements: carbon, oxygen, silicon, aluminum, calcium, and sulfur, more than 99% of the total mass of the coal. Among them, the carbon element content is as high as 80%, indicating that the coal contains a large amount of carbon-containing organic compounds, and the degree of carbonization is relatively high. Oxygen in coal is mainly present in various oxygen-containing compounds. More silicon and aluminum indicate that the coal sample may contain more kaolinite minerals or minerals such as quartz crystals. The high



Figure 2. Variations of typical element content in coal at different immersion time (the dotted line is the trend line)

content of calcium can infer that the sample contains a certain amount of calcite. The content of iron and sulfur is about 0.5%, indicating that a small amount of pyrite may be associated with the sample. There is less potassium, and the sample may contain very small amounts of orthoclase, illite, and other minerals.

Figure 2 shows the change curve of element content. Comparing the change trend of the content of each element in the coal sample with the increase in water immersion time, it is found that carbon element, oxygen element, and sulfur element basically remain unchanged, but there is a small margin fluctuations. The calcium element content shows a downward trend but suddenly rises after immersing for 20 days. The content of silicon and aluminum changes in the same trend, but slightly decreases. It is speculated that Al and Si in the sample are in the same mineral, so these two elements change identically with the water immersion time. At the same time, it can be seen that the content of Al and Si elements are decreasing in the element change curve of different immersion time. It is inferred that as the immersion time increases, the minerals containing silicon and aluminum in coal continue to separate from the matrix and dissolved in water; minerals containing oxygen and sulfur have a upward trend under the influence of the decrease in the content of other types of minerals.

The content of coal samples with different immersion time

The mineral composition analysis of coal samples with different immersion time adopts XRD method, and the sample preparation is similar to elemental analysis.

The main inorganic components of coal with different immersion time are kaolinite and calcite obtained by XRD pattern. Figure 3 shows the content of kaolinite and calcite varies with the time of immersion.

Analyze the mineral composition of coal samples with different immersion time, and obtain the main inorganic mineral components of coal samples with different immersion time. The final analysis shows that in addition carbon-containing organic matter in the sample coal matrix, the inorganic matter mainly con-



Figure 3. Changes in the content of main mineral components of coal at different immersion time (the dotted line is the trend line)

tains kaolinite and calcite two kinds of mineral crystals. Some samples contain dolomite, iron dolomite and calcium carbonate minerals, of which the relative content of kaolinite is the highest, mostly reaching over 80%, followed by calcite. This section will focus on the changes in the content of kaolinite and calcite, the main mineral components in coal. From fig. 3, it can be concluded that with the increase of immersion time, the kaolinite content of the coal sample shows an overall increasing trend, while the calcite content shows a decreasing trend. The Mohs hardness of kaolinite and calcite contained in coal are 2~2.5 and 3~3.5. The hardness of calcite is generally higher than that of kaolinite and other carbon-containing organic matter in coal matrix, and its brittleness is also greater. Coal is affected by hydration, hydrolysis and dissolution, etc., and harder mineral particles such as calcite are easy to fall off and form fine pore cracks. Therefore, as the immersion time increases, the strength of coal samples generally shows a downward trend. In addition, the main component of calcite mineral is calcium carbonate. Calcite continuously dissolves to form calcium bicarbonate, which is dissolved in water. Under the combined action of the aforementioned two factors, as the immersion time increases, the content of calcite in the coal decreases, causing the proportion of kaolinite to rise relatively. At the same time, the chemical formula of kaolinite is Al₂(Si₂O₅)(OH)₄, which verifies the speculation that aluminum and silicon are in the same mineral in the previous elemental analysis test. The XRD test result analysis is consistent with the element content analysis result.

Analysis of micro-structure of coal at different immersion time

There are a large number of pores and joint fissures in the coal mass [26]. The filling of moisture in the pores and fissures of the coal will inevitably change its mechanical properties. This chapter mainly uses NMR and SEM to analyze the pore structure of coal samples and observe the microscopic characteristics of the fractures, and explore the fracture characteristics and mechanisms of coal at different immersion time.

Analysis of pore structure of coal with different immersion time based on NMR

The NMR core analysis system uses the Oxford instrument GeoSpec2/150 (UK). The system is mainly used to predict the basic physical parameters of the rock, such as porosity and pore size distribution, free and bound fluid determination and T_2 cut-off value.

The relaxation characteristic is expressed [27]:

$$\frac{1}{T_2} \approx \rho_2 \left(\frac{S}{V}\right) = F_s \frac{\rho_2}{r} \tag{4}$$

where T_2 is the transverse relaxation time, ρ_2 – the surface relaxation rate, S – the surface area of pores, V – the volume of fluid, F_s – the geometric factor, and r – the pore radius. Therefore, there is a fixed corresponding relationship between T_2 value and porosity. The larger T_2 is, the larger the corresponding pore radius is. The size of NMR signal can reflect the water content corresponding to different T_2 values [28].



Figure 4. The *T*₂ spectrum distribution of coal samples with different immersion time

Figure 4 shows the T_2 distribution map of coal with different immersion time. On the whole, the effective signal T_2 of samples with different immersion time is between 0.01 ms and 1000 ms, and there are three peaks. The relaxation time increases from left to right and there are three peaks are roughly distributed in 0.01~3ms, 3~45ms, and 45~1000 ms, corresponding to micropores, mesopores and macropores, respectively. In some working conditions, the boundary between mesopores and

macropores is not obvious. From the peak distribution of the T_2 map of the coal sample, the proportion of micropores is the largest, followed by mesopores, and the proportion of macropores is the smallest.

Figure 5 shows the evolution of the cumulative porosity of pores of different sizes in the T_2 spectrum obtained by NMR measurement of coal samples with water immersion time. It can be seen that the porosity measured by NMR first increased and then decreased and then in-



Figure 5. Pore evolution of coal samples with different water immersion time

creased, the micropores first increased and then decreased, the mesopores continued to increase, and the macropores rose in a fluctuating manner, on the whole, the percentage of micropores showed a decreasing trend, and the mesopores and macropores showed an increasing trend. It indicating that the diameter of pores in coal gradually increases as a whole, and new pores are continuously generated at the same time. Internal cracks continue to develop and expand,

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and the type of pores changes in the direction of new pores or micropores to mesopores and macropores.

The coal sample was tested by NMR and the measured signal comes from the hydrogen protons in the pore moisture. The signal strength represents the moisture content. Therefore, the accumulated porosity in a certain relaxation time period is proportional to the amount of fluid contained in the rock. The overall change trend of coal porosity is basically consistent with the change curve of isothermal immersion moisture content. In the early stage, it increased rapidly with the increase of immersion time, and then the growth rate slowed down and gradually stabilized. The coal is basically saturated after 20 days of natural immersion. Therefore, the NMR test results with the immersion time of less than 20 days mainly reflect the specific process of the moisture in the coal gradually filling the pores of the coal. At this time, the porosity continues to rise because the coal sample is not saturated; the moisture content continues to rise. The permeability of coal samples decreases between two days and 10 days after immersion in water. According to the results of SEM, it is inferred that the pores are reduced due to the peeling of more layered and flaky coal, and after 20 days of immersion, the test result focuses on the changing law of coal pore structure under the action of water. The permeability increases slightly after being saturated with water. At this time, some minerals are dissolved by the action of water dissolution, and the granular matrix falls off, and the material in the pores precipitates. Internal fissures continue to develop and expand, and micropores increase.

Combining with the law of pore size development of coal samples at different immersion time, it is inferred that before saturation, water quickly enters the pores of the sample, so the porosity of the macropores, mesopores, and micropores in the early stage continues to rise. When the immersion is close to saturation, it is easier for water to enter the mesopores and macropores with less bound moisture content, which makes the porosity of these two pores gradually increase. In addition, as the immersion time increases, various mineral components and carbon-containing organic matter in the coal sample absorb water and expand and soften due to the effects of water dissolution and hydrolysis, and them dissolved in water and small particles fall off, resulting in changes in the pore structure. Part of the micropores gradually developed into mesopores, and part of the original mesopores evolved into macropores.

It can be seen from figs. 4 and 5 that the NMR signal is still measured in the not immersed state. Although the peak is relatively small, it shows that there is still a small amount of moisture in the dry coal. Most of this moisture is distributed in the contact corners and fine pores of coal particles, or is adsorbed on the surface of the coal particle skeleton and cannot move freely, and this part of bound moisture is mainly distributed in the micropores with the largest proportion. The T_2 boundary value of movable fluid and bound fluid is called T_2 cut-off value, T_2c , which is the boundary between bound fluid and free fluid. It is generally believed that the fluid with a corresponding T_2 value greater than T_2c on the T_2 distribution spectrum is a movable fluid, and a fluid with a value less than T_2c is a bound fluid. The coal's petrological characteristics and pore-fissure structure characteristics are different, so its bound moisture state is also different. In this experiment, the NMR T_2c of the sample under different immersion time is 33 ms. There is a general rule in the T_2 spectrum of coal samples, that is, when the T_2c value of the coal sample is low (generally less than 10 ms), and there is no or only a small movable fluid peak in the T_2 spectrum, and such coal is generally dominated by the development of adsorption pores and the permeability is generally very low. When the T_2c value of the coal sample is high (generally greater than 10 ms), and there are obvious movable fluid peaks in the T_2 spectrum, especially the fissure water peak, and such coal is mainly developed with macropores and cracks, and its permeability is generally high [29].

Analysis of coal natural fracture by SEM with different water immersion time

The natural fracture morphology of coal at different immersion time was analyzed using the JSM-7500F SEM. Preparations before the test:

coal sample soaking and

coal sample drying.

Through SEM test of coal slices from Pingdingshan coal mine area at different immersion time, the natural fracture morphology, microscopic composition, and structural features of coal at different immersion time were observed and identified. The micro-structure of coal shows that it is mainly composed of coal matrix, cracks, pores and a large amount of debris. Referring to the typical characteristics corresponding to the main components of coal in coal petrology, it can be seen that the microscopic composition of coal samples is mainly vitrinite, and the vitrinite is dense and smooth, indicating that it is mainly unstructured vitrinite, the content of inert group is small, there are very few fusinite and chitosome, in addition, it also contains auto-crystalline or semi-crystalline minerals such as kaolinite. According to the characteristics of the microscopic components contained in coal, the coal is bright coal, its luster is inferior to that of vitrinite, the surface is more brittle, and fine textures are faintly visible on the surface, and the endogenous fissures are more developed but not as good as vitrinite.



Figure 6. Typical fractures and micro-structures of different water-immersed coals

According to the scanning results, the evolution process of coal fracture and microstructure with water immersion time is divided into six stages, fig. 6:

Water immersion time 0-3 hours: At this stage, the internal structure of the coal is dense, the pores are small and no connection between pores. Before being immersed in water, a large number of flakes and granular coal particles were attached to the stepped fractures and rough parts of the coal matrix. As the immersion time increases, micro-particles will precipitate, resulting in increased pores, larger pores, and deeper pore diameters. In addition, the

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layered and flake-like structure on the surface of the coal matrix is peeled off, and the coal matrix is relatively flat, and coal particles that have not been washed away are attached to the surface of the coal substrate.

- Water immersion time 3-12 hours: Under the action of water, the rough fracture surface becomes smooth, the coal sample stratification structure is obvious, and the fracture morphology is mainly conchoidal and step-like. Part of the granular structure existing in the coal precipitates and swells into spherical particles by absorbing water during the movement. At this stage, tension fissures are developed, vertical fractures with large drop and flat curved step cleavage appear.
- Water immersion time 12 hours-10 days: Flake, crushed coal and spherical coal particles reappear on the surface of the coal matrix, coal particles continue to precipitate, and the flake and crushed coal particles on the surface of the coal matrix continue to increase. Simultaneously micropores, holes, and layered cleavage reappear. The flake structure is obviously increased, and the crushed coal particles reduced. Larger coal particles are left, and there are more peeling marks of layered and flake coal. After that, the coal particles were further reduced, the materials in the pores were precipitated, the micropores were developed and expanded, and water erosion and flaking coal pieces were observed.
- Water immersion time 10-20 days: At this stage, the material in the pores is further precipitated, the pores develop and expand to form larger pores, the fracture surface becomes rough due to water dissolution, and the flaked coal pieces are larger. The cohesive force between fine-grained coals is weakened, coal particles and flakes are continuously precipitate from the coal matrix, the pores become larger, and the cracks become deeper.
- Water immersion time 20 days-1 month: The effects of water dissolution and exfoliation make the fracture surface more micropores. The clearance between the layers increases, the phenomenon of layer peeling occurs, and a larger area of fracture occurs inside the stratification. The thick layered coal flakes off to form a vertical fracture.
- Water immersion time 1 month-3 months: At this stage, special filamentous phenomena and uneven layered structure appear, the cohesive force between coal stratification is weakened, coal particles and calcite particles precipitate, and a large amount of broken pieces appear at the vertical fracture. For the sample, the fracture surface is rough, with micro-cracks at the bottom, and the permeability is enhanced.

Based on two different methods to analyze the micro-structure of coal samples, the proportion of micropores in the coal sample is the largest, followed by mesopores, and the smallest proportion of macropores. As the water immersion time increases, the internal structure of the coal sample changes. Due to the effects of water dissolution and hydrolysis, various mineral components and carbon-containing organic matter in the coal sample swell and soften by absorbing water, and the soluble matter and small particles fall off. As a result, the pore structure changes, some of the micropores gradually develop into mesopores, and some of the original mesopores evolve into macropores, and the permeability is enhanced, so as to reduce the probability of gas disaster [30, 31]. The longer the immersion time is, the more serious the internal matrix will peel off. The dissolution of water will erode the coal, weaken the cohesive force, peel off the broken coal, and lower the strength.

Conclusion

The coal sample in this mining area belongs to the coking coal under the bituminous coal category. The main inorganic substances are kaolinite and calcite. The content of kaolinite increases with the increase of water immersion time, while the content of calcite is opposite.

The change of mineral composition leads to the corresponding element content variety. In addition, due to the shedding of harder mineral particles such as calcite, micropores and cracks will be formed, which will reduce the strength of the coal sample. The proportion of micropores in the coal sample is the largest. With the increase of water immersion time, the fracture surface becomes rough, and the pore ratio of the coal sample first increases, then decreases and then increases. Under the action of water dissolution and hydrolysis, various types of the mineral composition and carbon-containing organic matter swell and soften by absorbing water. The material in the pores is precipitated, and the pore structure gradually develops and evolves. The longer the immersion time, the more serious the internal matrix will peel off, the broken coal will peel off, the bonding force will be weakened, and the permeability will increase. The differences in the characteristics of coal mineral composition, the distribution of pores and fissures have a great impact on the macro-mechanical properties of coal mass. This paper combines a variety of experimental methods to capture the evolution characteristics of coal samples' elements, composition and pore structure at different immersion time. The experimental results deeply understand the influence of water on the evolution of coal pore structure at different immersion time, and analyze the interaction mechanism between water and weak coal seams from a microscopic perspective, and provide guidance for safe and efficient mining of water-injected coal seams in Pingdingshan Coal Mine.

Acknowledgment

This work was financially funded by Open Research Fund of State Key Laboratory of Coking Coal Exploitation and Comprehensive Utilization, China Pingmei Shenma Group, Grant No. 41040220181107-1, Sichuan International Technological innovation Cooperation Project (2018HH0159), National Natural Science Foundation of China (U2013603, 52004167, 51827901, and U1965203), Shenzhen Fundamental Research Project (JCYJ20190808153416970).

Nomenclature

- A_{ad} mass fraction of ash, [%]
- F_s geometric factor, [–]
- M_{ad} mass fraction of moisture, [%]
- m_0 mass of the empty crucible, [g]
- m_1 weight of the coal sample, [g]
- m_2 mass of sample and crucible after heating, [g]
- m_3 mass of residue and crucible, [g]
- m_4 mass of residue and crucible, [g]

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- r pore radius, [nm] S – surface area of pores, [nm²]
- T_2 transverse relaxation time, [ms]
- V volume of fluid, [nm³]
- V_{ad} mass fraction of volatile, [%]

Greek symbol

- ρ_2 surface relaxation rate, [nm·ms⁻¹]
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Paper submitted: January 11, 2021 © 2021 Society of Thermal Engineers of Serbia Paper revised: March 18, 2021 Published by the Vinča Institute of Nuclear Sciences, Belgrade, Serbia. Paper accepted: April 24, 2021 This is an open access article distributed under the CC BY-NC-ND 4.0 terms and conditions