Study on the Wettability of a Composite Solution Based on Surface Structures of Coal

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ABSTRACT: In order to research the influence of composite surfactant solutions on the wetting ability of coal, the wettability parameters, pore structure parameters, and surface microscopic morphology were determined in this study. The results show that the wettability of the surfactant can be improved by adding NaCl. As the concentration of NaCl increased, the spreading coefficient of the NaCl–SDS composite solution increases; the spreading coefficient increased from −10.838 to −3.7624 mN/m. The surface free energy decreased from −2.031 to 3.670 J/mol × 10^3, and the adhesion work decreased from 113.802 to 55.058 mJ/m^2. In terms of the pore structure and surface morphology of coal, the pore size will affect the wettability of coal. The contact angle reduces with pore size increase (R^2 = 0.955). The surface pores of coal treated with the NaCl–SDS composite solution increase and the fracture connectivity is improved, which facilitated the solution to penetrate coal for wetting. The results of this paper have great practical significance for mining at the face to reduce coal dust pollution.

1. INTRODUCTION

China is one of the countries with the richest coal reserves in the world, and it is also a large coal energy consumer. In the next few years, coal will still be the main body of energy production and consumption in China. Coal dust is one of the five major hazards in coal mines. In the process of coal mining, excessive coal dust accumulation can easily cause disastrous explosions. In addition, small particles such as coal dust are easily inhaled into the body through the respiratory system and this long-term inhalation of coal dust can cause pneumoconiosis, which seriously threatens the health of coal miners. With the widespread application of mechanized coal mining in China, the amount of coal dust produced at coal seam faces has increased, and the probability of coal miners suffering from pneumoconiosis also increases. In recent years, pneumoconiosis has become the most serious occupational disease within coal mines in China. The safety of coal production has become an important link in the field of energy security in China.

In order to reduce the amount of coal dust at the working face and ensure the neatness of the coal seam face, spray dust reduction is currently used for wet dust removal. Generally, the liquid used in wet dust removal is water, but because of the hydrophobicity of the coal dust surface and the high surface tension of water, coal dust is difficult to wet down with water and the dedusting efficiency is low. Enhancing the wetting ability of water can improve the efficiency of spray dust removal. The unique amphiphilic molecular structure of surfactants makes them hydrophilic and lipophilic, and their hydrophilic properties play a decisive role in reducing the surface tension of water. Classification of surfactants according to the dissociation properties of polar groups includes anionic surfactants, cationic surfactants, amphoterotic surfactants, and nonionic surfactants. Li and Li studied the wetting mechanism of coal; the results show that the wetting ability of coal is related to the oxygen content, moisture, ash, and other factors. Li et al. systematically analyzed the physical properties and wetting behavior of coal dust, studied the influence of different surfactants on the wetting behavior of coal dust, and found that 0.2% concentration of SDS has the best wetting effect on coal dust. Meng et al. investigated the effect of different concentrations of SDBS on the wettability of coal dust by molecular dynamics simulation. It was found that the difference in the spatial distribution of alkane chains and benzene rings of surfactant molecules resulted in the difference in the wettability of SDBS (sodium dodecyl benzene sulfonate) on the surface of coal samples. The species, molecular structure, and chemical properties of surfactants are all factors
Scholars improve the wettability of a single surfactant by compounding the surfactant. Adding inorganic salts to surfactants can improve the wettability of surfactants on coal to a certain extent. Hagebeucker mixed MgCl2 and CaCl2 with nonionic surfactants for dust wetting. Chang et al. found that inorganic salts can electrostatically interact with surfactants to affect the adsorption capacity of surfactants on solid surfaces. The research of Kilau and Pahliman shows that potassium salt or sodium salt can improve the wetting ability of the anionic surfactant solution. Wang et al. compounded disodium salt to improve the wetting ability of anionic surfactants for dust wetting. Chang et al. found that inorganic surfactant. Adding inorganic salts to surfactants can improve the wettability of a single surfactant by compounding the surfactant. Wang et al. selected three kinds of anionic surfactants and six kinds of coal samples to study the influence of different kinds of surfactants on the wettability of different kinds of coal in terms of physical and chemical properties. The results show that the pore size of coal is related to the wetting ability of the coal. The larger the pore size, the smaller the contact angle. He et al. used FTIR and Raman spectroscopy to comprehensively characterize the chemical structure of lignite and anthracite to understand the physical and chemical properties of coal. Nie et al. studied the microscopic mechanism of coal adsorbing water, which laid a theoretical foundation for improving the wettability measures of coal seams.

Based on previous research, the influence of the NaCl−SDS composite solution on the wetting ability of coal was analyzed. The surface tension and contact angle of the NaCl−SDS composite solution were analyzed by the wettabilty parameter experiment. The wettabilty parameters (spreading coefficient, adhesion work, and surface free energy) of the solution were calculated with the contact angle and surface tension data to further evaluate the wettability of the NaCl−SDS composite solution. At present, research on the influence of surfactants on the pore structure of coal is relatively less. Therefore, the low-temperature liquid nitrogen experiment and scanning electron microscopy (SEM) were used to test the pore structure characteristics and micromorphology of coal samples treated with different solutions. In this paper, the variation in the wetting property parameters of composite solutions is investigated; the wetting property of composite solutions is evaluated, and the influence of the pore structure of coal treated with different-concentration solutions on the wetting ability of coal was analyzed. The results of this paper have great practical significance to reduce coal dust pollution.

2. RESULTS AND DISCUSSION

2.1. Analysis of Wettability Parameters. The surface tension and contact angle are the intuitive parameters to characterize the wettability of a solution. The surface tension is the pulling force between any two adjacent parts of the liquid surface, which is perpendicular to the boundary line of their unit length. The surface tension can directly reflect the wettability of the solution. The smaller the surface tension, the better the wettability of the solution. The tangent line is made at the intersection of the gas, liquid, and solid; the angle θ formed by the tangent line between the liquid side and the solid–liquid boundary is called the contact angle. The contact angle is an important parameter to characterize the wettability of a solution to the coal surface. The smaller the contact angle, the stronger the wettability of the solution. The wetting effect of water on coal is mainly caused by the mutual attraction between water molecules and the coal dust surface. Therefore, surfactants are usually added to water to reduce the surface tension of water and improve the wettability of water to coal. The surface tension and contact angle of four different concentrations of the NaCl−SDS composite solution are obtained through experiments, as shown in Figure 1. The surface tension of water is 72 mN/m at 298 K. The surface tension of the water is significantly reduced after adding the composite solution to the water. The results show that the surface tension and contact angle of the solution decreased with increased concentrations of the NaCl−SDS composite solution. Thus, the addition of NaCl to SDS solution is beneficial to enhance the wettability of a surfactant solution, and the wettability of a surfactant solution is enhanced with the increase in the NaCl concentration.

According to the experimental data, the surface tension and contact angle of the composite solution and the wettability parameters (spreading coefficient, adhesion work, and surface free energy) of the NaCl−SDS composite solution on the surface of coal samples were calculated to further evaluate the wettability of the NaCl−SDS composite solution. When the liquid drops onto the solid surface, the liquid–solid interface replaces the gas–solid interface, while the gas–liquid interface expands by the same area; this process is called spreading. A parameter “S” is defined as the spreading coefficient to measure the spreading capacity and wetting state of the solution on the solid surface. The difference in the spreading coefficient makes the wetting state of the system in the equilibrium state different. The larger the spreading coefficient of the solution, the stronger the spreading ability and the better the wetting ability. The spreading coefficient is related to three free energies in the spreading system, and its expression is:

$$S = \gamma_{GS} - \gamma_{SL} - \gamma_{GL}$$  \hspace{1cm} (1)

where, $\gamma_{GS}$, $\gamma_{SL}$, and $\gamma_{GL}$ are the surface tensions of the solid–gas, solid–liquid, and gas–liquid interfaces, respectively.
When a droplet reaches equilibrium on the solid surface, the relationship of the contact angle and $\gamma_{SG}, \gamma_{SL}$, and $\gamma_{GL}$ follows Young’s equation, which is expressed as\(^{42}\)

$$\gamma_{SG} - \gamma_{SL} = \gamma_{GL} \cos \theta$$  

(2)

Because it is difficult to measure the surface tension of the solid–gas and solid–liquid interface by experiments, the formula for the solution spreading coefficient is obtained by combining Young’s equation with Formula 1.

$$S = \gamma_{GL} (\cos \theta - 1)$$  

(3)

Adhesion work ($W_a$) refers to the work that needs to be done in the process of wetting the solid with a solution. The smaller the adhesion work, the less the work done by the solution in the process of wetting the coal and the solution finds it easier to wet the coal sample. The formula is as follows

$$W_a = \gamma_{SG} + \gamma_{SL} - \gamma_{GL} (\cos \theta + 1)$$  

(4)

Surface free energy refers to the thermodynamic function value corresponding to the unit area, which is the theoretical basis for studying the wettability of a solid surface. Both surface free energy and surface tension are physical quantities describing the surface state of an object. Surface free energy is a form of internal energy, and surface tension is a form of intermolecular force. It can be calculated according to the formula provided by EXTRAND\(^{57}\)

$$\Delta G = \frac{gT}{3} \ln \left[ \left( 1 - \cos \theta \right)^2 (2 + \cos \theta) \right]$$  

(5)

In the formula, $g$ is the ideal gas constant, 8.314 J/(mol·K), and $T$ is absolute temperature, 298 K.

According to the abovementioned formulas, the wettability parameters were calculated and the results are recorded in Table 1.

| Table 1. Wettability Parameters |
|--------------------------------|
| | solution number |
| **wettability parameters** | 1# | 2# | 3# | 4# |
| surface tension (mN/m) | 62.32 | 32.21 | 30.96 | 29.41 |
| contact angle (deg) | 34.3 | 33.8 | 32.5 | 29.3 |
| spreading coefficient (mN/m) | −10.838 | −5.4440 | −4.849 | −3.7624 |
| adhesion work (mJ/m²) | 113.802 | 58.976 | 57.071 | 55.058 |
| surface free energy (J/mol × 10¹⁴) | −2.031 | −3.222 | −3.344 | −3.670 |

The variation in the spreading coefficient and surface free energy is shown in Figure 2. The spreading coefficient, surface free energy, and NaCl concentration were linearly fitted, and the results are shown in Table 2. It can be seen from the fitted results and the change images that the spreading coefficient had a positive correlation with the concentration of NaCl, while the surface free energy had a negative correlation with the concentration of NaCl. The spreading coefficient gradually increased and tended to be stable. The surface free energy gradually decreased.

According to the formula for the spreading coefficient and surface free energy, the increase in the spreading coefficient is mainly related to the decrease in the surface tension and contact angle of the NaCl–SDS composite solution, and the surface free energy is related to the contact angle. It can be seen from Figure 1 that with the increase in NaCl concentration in the NaCl–SDS composite solution, the surface tension and contact angle show a decreasing trend, which indicates that adding a certain amount of inorganic salt to the surfactant can improve the surface activity of the surfactant. Previous studies have shown that adding NaCl to SDS can increase the Krafft value of the surfactant and reduce the critical micelle concentration, thus enhancing the ability of the surfactant to reduce the surface tension of the solution. There is a strong electrostatic field around the ionic surfactant group, and the electrostatic repulsion between surfactants is not conducive to the aggregation of surfactant molecules. NaCl has a certain effect on the aggregation of surfactant molecules. The counterions in the NaCl are attracted to the surfactant ions because of the influence of the overlapping electric field of the surfactant ions, which plays an electrical neutralizing role on the surfactant and reduces the electrostatic repulsion between the SDS molecules. It is beneficial to the aggregation of surfactant molecules and reducing the surface tension of the solution. The change process is shown in Figure 3. The tensile force of liquid surface molecules is called the surface tension. When the surface tension decreases, the tensile force of liquid surface molecules weakens accordingly, which makes the solution spread easily on the surface of the coal sample and increases the contact between the solution and the coal sample. Thus, the contact angle decreases. The decrease in the surface tension and contact angle makes the spreading coefficient increase. That is, adding NaCl can promote the spread of the surfactant solution on the coal surface, and it is easier to wet the coal sample. In addition, we speculate that there will be synergism between NaCl and SDS, which will promote the spread of the SDS surfactant solution on the solid surface. The surface tension, contact angle, and surface free energy of the NaCl–SDS composite solution decrease because of adsorption at the solid–liquid interface and gas–liquid interface. The abovementioned analysis shows that the wetting effect of the surfactant was enhanced with the increase in NaCl concentration in the NaCl–SDS composite solution.
As shown in Figure 4, the adhesion work gradually decreased and tended to be stable. Its change trend conforms to the rule of exponential function. The adhesion work is the amount of work that the solution did wetting the coal sample. The decrease in the adhesion work indicates that the work done by the NaCl−SDS composite solution in the process of wetting the coal sample reduced. The “salt bridge” can be formed between the NaCl and SDS; Na+ as the “salt bridge” is connected with the head group of anionic surfactants and plays an important role in stabilizing the structure of the SDS micelles.60 Na+ makes the counterions gather around the surfactant molecules, thus making the arrangement of the surfactant molecules more compact and forming a strong monolayer adsorption layer. The enhancement of the interaction force between the hydrophobic group of surfactant molecules and the coal sample surface makes the solid−liquid interfacial tension decrease and increases the affinity between the solution and the coal sample. The spread of the surfactant solution on the coal sample surface is promoted. The solid surface of coal dust attracts the liquid molecules and makes the surfactant wet the coal. When the attractive force between the NaCl−SDS composite solution and coal dust is greater than the repulsive force, the process of wetting the coal sample with the NaCl−SDS composite solution is easier, that is, the adhesion work is reduced.

2.2. Influence of the Pore Structure on the Wetting Ability of Coal Dust. Coal dust wetting is a complex process, which involves the result of solid−liquid−gas interactions.51 Not only do the material composition and chemical structure of coal itself promote the wetting effect but also the pore structure of the coal will affect the wetting ability of coal.61 The pore structure of the coal sample is small, the surfactant molecule cannot enter the pore from the surface of coal, the wetting of surfactant solution to the coal sample can only occur on the surface, and the wetting effect is poor. When the coal sample has a large pore structure, the stronger the adsorption capacity of the coal sample to the surfactant solution is, so it is easier to wet the coal. Treating coal samples with different concentrations of the composite solution may change the pore structure of the coal and affect the wetting ability of coal dust. To analyze the relationship between the pore structure and wetting ability of coal dust, the pore structure of coal was tested using the ASAP2460 automatic surface area and porosity analyzer with low-temperature liquid nitrogen adsorption.

According to the experimental data of low-temperature liquid nitrogen adsorption, Brunauer−Emmett−Teller (BET) polylayer adsorption theory was used to obtain the surface area and pore size of coal samples, and the Barrett−Joyner−Halenda (BJH) model was used to calculate the pore volume distribution. The surface area, the pore size, and the most probable pore diameter of coal samples are shown in Table 3. As shown in Table 3, the pore structure data of coal changed after treatment with different concentrations of the composite solution. The pore size and the most probable pore diameter of coal samples have shown a tendency from small to large, while the surface area decreased with the increase in the coal pore.
From this, we speculated that the pore structure of coal will be affected when the coal sample was treated with the composite solution, which makes some small pores expand into mesopores. Therefore, the pore size and the most probable pore diameter of coal have shown an increasing trend.

In order to further analyze the effect of the pore structure on the wetting ability of coal, the surface area and pore size of coal samples were fitted with the contact angle. The fitting results and formulas are shown in Figure 5 and Table 4, respectively.

The correlation between the surface area and the contact angle was small, and the correlation coefficient $R^2 = 0.663$, which shows a positive correlation change. The larger the surface area, the larger the contact angle. The pore size was negatively correlated with the contact angle. The larger the pore size, the smaller the contact angle. This is because the larger the pore size of coal samples, the more favorable it is for the surfactant molecules to invade coal samples, and it can effectively reduce the resistance to be overcome when the NaCl–SDS composite solution contacts the coal samples. The adhesion work needed to be done in the process of wetting coal samples is reduced, which makes the NaCl–SDS composite solution easier to spread on the surface of the coal samples and the contact angle decreases. It is beneficial to the wetting of coal samples. When the pore size of the coal samples is small, the wetting effect of the NaCl–SDS composite solution on the coal samples only occurs on the surface. It is difficult for surfactant molecules to enter the coal sample, and the contact angle is large and the wetting effect is poor. Among the pore structures of coal, the pore size distribution of coal samples obtained by the BJH method is shown in Figure 6. It can be seen from Figure 6 that the pore size of the four coal samples was mostly between 2 and 20 nm, and the mesopore distribution was the most abundant. Although there was a number of micropores in the coal sample A and B, the micropore distribution in the coal sample C and D was obviously reduced and the distribution of mesopores was increased. Therefore, we speculated that soaking coal samples with a higher concentration of the composite solution can

Table 3. Pore Structure Date

| coal sample | surface area (m$^2$/g) | pore size (nm) | most probable pore diameter (nm) |
|-------------|------------------------|---------------|----------------------------------|
| A           | 16.1199                | 4.0786        | 3.50244                          |
| B           | 11.4501                | 4.5714        | 4.05725                          |
| C           | 5.0449                 | 7.9127        | 4.17594                          |
| D           | 4.4832                 | 11.0933       | 7.16117                          |

Figure 5. Effect of the pore structure on the contact angle.

Table 4. Fitting of the Surface Area and Pore Size

|         | fitting formula | correlation coefficient ($R^2$) |
|---------|----------------|-------------------------------|
| pore size | $y = 52.70 - 1.42x$ | 0.955                         |
| surface area | $y = -55.991 + 2.01x$ | 0.663                         |

Figure 6. Pore diameter distribution of the coal samples.
enlarge the pore size and increase the distribution of mesopores. The increase in the mesopore distribution is more conducive to the penetration of the NaCl−SDS composite solution into coal samples for wetting, making the wetting result tend to be in a positive direction. It can be seen from the abovementioned analysis that the increase in pore size and the decrease in contact angle are beneficial to the wetting of coal samples. Therefore, adding a higher concentration of NaCl to the surfactant solution to treat coal samples will cause differences in the pore structure of coal samples, leading to the differences in wettability and making the surfactant solution more easily wet the coal samples.

2.3. SEM and Energy Spectrum Analysis. To further analyze the effect of the NaCl−SDS composite solution on the coal pore structure and mineral elements, the surface morphology of coal samples was observed by SEM, and the migration of various minerals on the surface of the coal samples was measured using an energy-dispersive spectrometer.

Figure 7 shows the SEM photos of the coal samples treated with different concentrations of the solution magnified 2000 times; it is found that some minerals were attached to the coal sample surface, and the coal sample surface were rough. The surface of the coal sample A had more mineral distribution and less pore distribution, and the surface was the mostly rough. The image of the surface of the coal sample B was similar, but there were longer cracks and the surface had a small amount of minerals filled in the cracks. The surface of the coal sample C had more pores and the cracks were well-developed. There was no mineral filled between the cracks, and the connectivity is better than that of the coal samples A and B. The surface of the coal sample D had kaolinite protruding, and lots of intercrystalline pores were formed between the fragments. At the same time, fractures were formed into linear tension fractures with no minerals found inside the fractures. The fracture surface was relatively smooth and flat. The surface cracks can be connected with each other, and the pore connectivity is better. It can be seen from SEM that the main difference in the microscopic morphology of coal samples soaking in different solutions is cracks and pores. Compared with the coal samples treated only with SDS solution, the coal samples treated with the NaCl−SDS composite solution show more pore structures, the pores on the surface of coal samples increased, and the fracture connectivity became better. The pore and fracture structure of coal play an important role in the process of coal wetting. The more pore structure found in the coal, the better the fracture connectivity, which is beneficial for the NaCl−SDS composite solution to penetrate the coal samples and easier than to wet the coal. Furthermore, a rough surface makes the NaCl−SDS composite solution more difficult to spread on the surface of the coal sample, which makes the coal sample difficult to be wetted by the solution.

Coal is composed of organic matter and inorganic minerals, in which inorganic minerals are hydrophilic. The main mineral elements on the coal surface are carbon, oxygen, aluminum, silicon, and iron, which form the mineral crystals with clay, sulfide, carbonate, and silicon oxide as the main components attached to the surface and pore cracks of coal samples. Figure 8 shows the surface mineral map of coal samples after treatment with different concentrations of the composite solution. According to the energy spectrum analysis data, the
main substances on the surface of the four coal samples are SiO$_2$ and Al$_2$O$_3$. These two substances are the main components of clay; therefore, the main minerals attached to the surface of coal samples are clay, which is a kind of hydrophilic mineral. The hydrophilic minerals attached to the surface and cracks of coal samples will make the NaCl–SDS composite solution more likely to invade the coal samples, which is conducive to wet coal samples. In addition, it is found that the surface of the four coal samples contains carbon, oxygen, aluminum, silicon, and other elements, and their contents have not changed significantly. Therefore, we speculated that the treatment of coal samples with the composite solution will not damage the mineral elements contained in the coal samples.

3. CONCLUSIONS
To research the effect of the NaCl–SDS composite solution on the wetting ability of coal, the surface tension and contact angle of the solution were obtained by wettability parameter experiments. Additionally, the wettability parameters (spreading coefficient, surface free energy, and adhesion work) of the solution were calculated to evaluate the ability of the NaCl–SDS composite solution to wet coal dust. The pore structure and surface microscopic morphology of coal were analyzed by the low-temperature liquid nitrogen adsorption experiment and SEM. Combined with the contact angle, the effect of the pore structure on the wetting ability of coal was studied. The main conclusions are as follows:

1. The addition of NaCl to the SDS solution can improve the wettability of a single SDS solution on the coal sample. As the surface tension and contact angle of the solution decrease, the spreading coefficient of the solution increases, the surface free energy decreases, the solution is easier to spread on the surface of the coal sample, and the adhesion work required to wet the coal sample is reduced. Additionally, the effect is more significant with the increase in NaCl concentration in the NaCl–SDS composite solution.

2. Pore size is an important factor affecting the wetting ability of coal samples. The contact angle decreases linearly with pore size increase, and its linear correlation coefficient $R^2 = 0.955$. The pore structure of coal may be affected by soaking coal samples with the composite solution. The pore size of coal soaked in a solution containing a higher concentration of NaCl increases, which is beneficial to wetting coal dust.

3. The microscopic morphology of coal has a certain effect on the wettability of coal dust. The internal fracture of coal samples is well developed and the strong connectivity is favorable for the NaCl–SDS composite solution to invade coal samples for wetting.

4. MATERIALS AND METHODS
4.1. Preparation of Solutions. Hygroscopic inorganic salt can absorb the moisture in the surrounding air, causing the coal dust to retain a certain degree of humidity making it less easy to fly. Coal miners often add a small amount of inorganic salt to the dedusting agent to improve the wettability of the solution. In order to determine the effect of NaCl on the wetting ability of the SDS solution, the NaCl solution with a concentration of 0, 0.3, 0.6, and 0.9 mol/L was added into the SDS solution to make the NaCl–SDS composite solution. The concentration of the SDS solution was fixed at 6 × 10$^{-3}$ mol/L. The composite solutions were numbered 1#, 2#, 3#, and 4#.

4.2. Wettability Parameters Experiment. Dry lignite with a particle size of 200 mesh was selected, and the coal samples were made into cylindrical coal sheets with a thickness of 1 mm using a table pulverized coal press under a pressure of 15 MPa. The DSA25 optical droplet morphology analysis system manufactured by the German Kruss company was used to measure the contact angle between the composite solution and the coal sample. At the same time, the surface tension of four different concentrations of the composite solution was measured by the suspension drop method.

4.3. Low-Temperature Liquid Nitrogen Adsorption Experiment. Four parts of lignite with 60–80 diameter were weighed and immersed in the NaCl–SDS composite solutions numbered 1#, 2#, 3#, and 4#. After soaking for 24 h, the coal sample was separated from its supernatant and was neutralized by washing with distilled water. The coal sample was then
placed in a drying oven at 80 °C for 12 h to exclude the influence of moisture on the test results. The coal samples were numbered A, B, C, and D. The low-temperature liquid nitrogen adsorption experiment was measured using the ASAP2460 automatic surface area and porosity analyzer produced by Micromechanics Instruments Co. Ltd.

4.4. Scanning Electron Microscopy. The pore characteristics and mineral variation law of the coal sample surface were measured using SEM and an energy-dispersive spectrometer. The type of the scanning electron microscope used in the experiment was the Quanta TM 250. Acceleration voltage: 200 V to 30 kV, probe current: continuously adjustable less than or equal to 200 nA, and magnification: 6 to 10⁴ times. The experimental equipment and flow chart are shown in Figure 9.

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Notes

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■ NOMENCLATURE

\( \theta \) contact angle

\( \gamma_{SA} \) surface tension of the solid–gas interfaces

\( \gamma_{SL} \) surface tension of the solid–liquid interfaces

\( \gamma_{GL} \) surface tension of the gas–liquid interfaces

\( S \) spreading coefficient

\( W_a \) adhesion work

\( \Delta G \) spreading free energy

\( \gamma \) gas constant

\( T \) absolute temperature

■ REFERENCES

(1) Zhou, G.; Ding, J.; Ma, Y.; Li, S.; Zhang, M. Synthesis and performance characterization of a novel wetting cementing agent for dust control during conveyor transport in coal mines. Powder Technol. 2020, 360, 165–176.

(2) Wang, L.; Chen, Z.; Wang, C.; Elsworth, D.; Liu, W. Reassessment of coal permeability evolution using steady-state flow methods: The role of flow regime transition. Int. J. Coal Geol. 2019, 211, 103210.

(3) Xiu, Z.; Nie, W.; Chen, D.; Yan, J.; Cai, P.; Liu, Q.; Wei, C. Numerical simulation study on the coupling mechanism of composite-source airflow-dust field in a fully mechanized caving face. Powder Technol. 2019, 356, 443–457.

(4) Cai, P.; Nie, W.; Chen, D.; Yang, S.; Liu, Z. Effect of air flowrate on pollutant dispersion pattern of coal dust particles at fully mechanized mining face based on numerical simulation. Fuel 2019, 239, 623–635.

(5) Xiu, Z.; Nie, W.; Yan, J.; Chen, D.; Cai, P.; Liu, Q.; Du, T.; Yang, B. Numerical simulation study on dust pollution characteristics and optimal dust control air flow rates during coal mine production. J. Clean. Prod. 2020, 248, 119197.

(6) Bao, Q.; Nie, W.; Liu, C.; Zhang, H.; Wang, H.; Jin, H.; Yan, J.; Liu, Q. The preparation of a novel hydrogel based on crosslinked polymers for suppressing coal dusts. J. Clean. Prod. 2020, 249, 119343.

(7) Hua, Y.; Nie, W.; Liu, Q.; Peng, H.; Wei, W.; Cai, P. The development and application of a novel multi-radial-vortex-based ventilation system for dust removal in a fully mechanized tunnelling face. Tunn. Undergr. Space Technol. 2020, 98, 103253.

(8) Lu, S.; Zhang, Y.; Sa, Z.; Si, S.; Shu, L.; Wang, L. Damage-induced permeability model of coal and its application to gas predrainage in combination of soft coal and hard coal. Energy Sci. Eng. 2019, 7, 1352–1367.

(9) Lu, S.; Zhang, Y.; Sa, Z.; Si, S. Evaluation of the effect of adsorbed gas and free gas on mechanical properties of coal. Environ. Earth Sci. 2019, 78, 218.

(10) Yan, F.; Lin, B.; Xu, J.; Wang, Y.; Zhang, X.; Peng, S. Structural evolution characteristics of middle-high rank coal samples subjected to high-voltage electrical pulse. Energy Fuels 2018, 32, 3263–3271.

(11) Jingna, X.; Jun, X.; Guanhua, N.; Rahman, S.; Qian, S.; Hui, W. Effects of pulse wave on the variation of coal pore structure in pulsating hydraulic fracturing process of coal seam. Fuel 2020, 264, 116906.

(12) Guanhua, N.; Kai, D.; Shang, L.; Qian, S.; Dongmei, H.; Ning, W.; Yanying, C. Development and performance testing of the new sealing material for gas drainage drilling in coal mine. Powder Technol. 2020, 363, 152–160.

(13) Peng, H.; Nie, W.; Liu, Z.; Xiu, Z.; Yang, S.; Xu, C.; Ma, Q.; Guo, C. Optimization of external spray negative-pressure mist-curtain dust suppression devices for roadheaders based on a multi-factor orthogonal experiment. J. Clean. Prod. 2020, 275, 123603.

(14) Du, T.; Nie, W.; Chen, D.; Xiu, Z.; Yang, B.; Liu, Q.; Guo, L. CFD modeling of coal dust migration in an 8.8-meter-high fully mechanized mining face. Energy 2020, 212, 118616.

(15) Ma, Q.; Nie, W.; Yang, S.; Xu, C.; Peng, H.; Liu, Z.; Guo, C.; Cai, X. Effect of spraying on coal dust diffusion in a coal mine based on a numerical simulation. Environ. Pollut. 2020, 264, 114717.
(16) Yuan, M.; Nie, W.; Zhou, W.; Yan, J.; Bao, Q.; Guo, C.; Tong, P.; Zhang, H.; Guo, L. Determining the effect of the non-ionic surfactant AEO9 on lignite adsorption and wetting via molecular dynamics (MD) simulation and experiment comparisons. Fuel 2020, 278, 118339.

(17) Petavratzi, E.; Kingman, S.; Lowndes, I. Particulates from mining operations: A review of sources, effects and regulations. Miner. Eng. 2005, 18, 1183–1199.

(18) Wang, G.; Jiang, C.; Shen, J.; Han, D.; Qin, X. Deformation and water transport behaviors study of heterogenous coal using CT-based 3D simulation. Int. J. Coal Geol. 2019, 211, 103204.

(19) Wang, G.; Qin, X.; Shen, J.; Zhang, Z.; Han, D.; Jiang, C. Quantitative analysis of microscopic structure and gas seepage characteristics of low-rank coal based on CT three-dimensional reconstruction of CT images and fractal theory. Fuel 2019, 256, 115900.

(20) Wang, G.; Shen, J.; Liu, S.; Jiang, C.; Qin, X. Three-dimensional modeling and analysis of macro-pore structure of coal using combined X-ray CT imaging and fractal theory. Int. J. Rock Mech. Min. Sci. 2019, 123, 104082.

(21) Guanhua, N.; Zhao, L.; Qian, S.; Shang, L.; Kai, D. Effects of [Bmim][Cl] ionic liquid with different concentrations on the functional groups and wettability of coal. Adv. Powder Technol. 2019, 30, 610–624.

(22) Shi, S.; Jiang, B.; Meng, X.; Yang, L. Fuzzy fault tree analysis for gas explosion of coal mining and heading faces in underground coal mines. Adv. Mech. Eng. 2018, 10, 168781401879231.

(23) Li, S.; Zhou, G.; Wang, Y.; Jing, B.; Qi, Y. Synthesis and characteristics of fire extinguishing gel with high absorption water for coal mines. Process Saf. Environ. Prot. 2019, 125, 207–218.

(24) Zhang, Q.; Zhou, G.; Qian, S.; Xuan, M.; Sun, Y.; Wang, D. Diffuse pollution characteristics of respirable dust in fully-mechanized mining face under various velocities based on CFD investigation. J. Clean. Prod. 2018, 184, 239–250.

(25) Li, H.; Shi, S.; Lu, J.; Ye, Q.; Lu, Y.; Zhu, X. Pore structure and multifractal analysis of coal subjected to microwave heating. Powder Technol. 2019, 346, 97–108.

(26) Li, H.; Shi, S.; Lin, B.; Lu, J.; Lu, Y.; Ye, Q.; Wang, Z.; Hong, Y.; Zhu, X. A fully coupled electromagnetic, heat transfer and multiphase porous media model for microwave heating of coal. Fuel Process. Technol. 2019, 189, 49–61.

(27) Xu, C.; Wang, D.; Wang, H.; Ma, L.; Zhu, X.; Zhu, Y.; Zhang, Y.; Liu, F. Experimental investigation of coal dust wetting ability of anionic surfactants with different structures. Process Saf. Environ. Prot. 2019, 121, 69–76.

(28) Zhao, L.; Guanhua, N.; Lulu, S.; Qian, S.; Shang, L.; Kai, D.; Jingna, X.; Gang, W. Effect of ionic liquid treatment on pore structure and fractal characteristics of low rank coal. Fuel 2020, 262, 116513.

(29) Jingna, X.; Guanhua, N.; Hongchao, X.; Shang, L.; Qian, S.; Kai, D. The effect of adding surfactant to the treating acid on the chemical properties of an acid-treated coal. Powder Technol. 2019, 356, 263–272.

(30) Hongchao, X.; Guanhua, N.; Shang, L.; Qian, S.; Kai, D.; Jingna, X.; Gang, W.; Yixin, L. The influence of surfactant on pore fractal characteristics of composite acidized coal. Fuel 2019, 253, 741–753.

(31) Guanhua, N.; Hongchao, X.; Shang, L.; Qian, S.; Dongmei, H.; Yanying, C.; Ning, W. The effect of anionic surfactant (SDS) on pore-fracture evolution of acidized coal and its significance for coalbed methane extraction. Adv. Powder Technol. 2019, 30, 940–951.

(32) Chen, H.; Feng, Q.; Long, R.; Qi, H. Focusing on coal miners’ occupational disease issues: A comparative analysis between China and the United States. Saf. Sci. 2013, 51, 217–222.

(33) Zhou, W.; Nie, W.; Liu, C.; Liu, Q.; Hetang, W.; Wei, C.; Yan, J.; Yin, S.; Xiu, Z.; Xu, C. Modelling of ventilation and dust control effects during tunnel construction. Int. J. Mech. Sci. 2019, 160, 358–371.

(34) Liu, Q.; Nie, W.; Hua, Y.; Jia, L.; Li, C.; Ma, H.; Wei, C.; Liu, C.; Zhou, W.; Peng, H. A study on the dust control effect of the dust extraction system in TBM construction tunnels based on CFD computer simulation technology. Adv. Powder Technol. 2019, 30, 2059–2075.

(35) Yin, S.; Nie, W.; Liu, Q.; Hua, Y. Transient CFD modelling of space-time evolution of dust pollutants and air-curtain generator position during tunneling. J. Clean. Prod. 2019, 239, 117924.

(36) Liu, Q.; Nie, W.; Hua, Y.; Peng, H.; Liu, C.; Wei, C. Research on tunnel ventilation systems: Dust Diffusion and Pollution Behaviour by air curtains based on CFD technology and field measurement. Build. Environ. 2019, 147, 444–460.

(37) Xu, C.; Nie, W.; Liu, Z.; Peng, H.; Yang, S.; Liu, Q. Multi-factor numerical simulation study on spray dust suppression device in coal mining process. Energy 2019, 182, 544–558.

(38) Wang, J.; Zhou, G.; Wei, X.; Wang, S. Experimental characterization of multi-nozzle atomization interference for dust reduction by hydraulic supports at a fully mechanized coal mining face. Environ. Sci. Pollut. Res. 2019, 26, 10023–10036.

(39) Chen, Y.; Xu, G.; Huang, J.; Eksteen, J.; Liu, X.; Zhao, Z. Characterization of coal particles wettability in surfactant solution by using four laboratory static tests. Colloids Surf., A 2019, 567, 304–312.

(40) Wang, P.; Li, R.; Tang, M.; Zhang, W.; Gou, Z. Experimental study on atomization characteristics and dust suppression efficiency of high-pressure spray in underground coal mine. Meitan Xuebao 2015, 40, 2124–2130.

(41) Wang, P.; Tan, X.; Zhang, L.; Li, Y.; Liu, R. Influence of particle diameter on the wettability of coal dust and the dust suppression efficiency via spraying. Process Saf. Environ. Prot. 2019, 132, 189–199.

(42) Guanhua, N.; Qian, S.; Meng, X.; Hui, W.; Yuhang, X.; Weimin, C.; Gang, W. Effect of NaCl-SDS compound solution on the wettability and functional groups of coal. Fuel 2019, 257, 116077.

(43) Li, J. Y.; Li, K. Q. Influence factors of coal surface wettability. Meitan Xuebao 2016, 41, 448–453.

(44) Li, Q.; Lin, B.; Zhao, S.; Dai, H. Surface physical properties and its effects on the wetting behaviors of respirable coal mine dust. Powder Technol. 2013, 233, 137–145.

(45) Meng, J.; Yin, F.; Li, S.; Zheng, R.; Sheng, Z.; Nie, B. Effect of different concentrations of surfactant on the wettability of coal by molecular dynamics simulation. Int. J. Min. Sci. Technol. 2019, 29, 577–584.

(46) Guo, J.; Zhang, L.; Liu, S.; Li, B. Effects of hydrophilic groups of nonionic surfactants on the wettability of lignite surface: Molecular dynamics simulation and experimental study. Fuel 2018, 231, 449–457.

(47) Hagebeucker, K. Dust binder containing magnesium chloride and/or calcium chloride and perfume. Chem. Abstr. 1999, 130, 1002.

(48) Chang, Z.; Chen, X.; Peng, Y. The adsorption behavior of surfactants on mineral surfaces in the presence of electrolytes - A critical review. Miner. Eng. 2018, 121, 66–76.

(49) Kilau, H. W.; Pahlman, J. E. Coal wetting ability of surfactant solutions and the effect of multivalent anion additions. Colloids Surf. A 1987, 26, 217–242.

(50) Wang, K.; Ma, X.; Jiang, S.; Wu, Z.; Shao, H.; Pei, X. Application study on complex wetting agent for dust-proof after gas drainage by outburst seams in coal mines. Int. J. Min. Sci. Technol. 2016, 26, 669–675.

(51) Wang, X.; Yuan, S.; Jiang, B. Experimental investigation of the wetting ability of surfactants to coals dust based on physical chemistry characteristics of the different coal samples. Adv. Powder Technol. 2019, 30, 1696–1708.

(52) He, X.; Liu, X.; Nie, B.; Song, D. FTIR and Raman spectroscopy characterization of functional groups in various rank coals. Fuel 2017, 206, 555–563.

(53) Nie, B. S.; He, X. Q.; Wang, E. Y.; Zhang, L. Micro-mechanism of coal adsorbing water. Zhongguo Kuangye Daxue Xuebao 2004, 33, 379–383.

(54) Zhou, G.; Qiu, H.; Zhang, Q.; Xu, M.; Wang, J.; Wang, G. Experimental investigation of coal dust wettability based on surface contact angle. J. Chem. 2016, 2016, 1–8.
Mirchi, V.; Saraji, S.; Goual, L.; Piri, M. Dynamic interfacial tension and wettability of shale in the presence of surfactants at reservoir conditions. *Fuel* 2015, 148, 127–138.

Si, Y.; Yu, C.; Dong, Z.; Jiang, L. Wetting and Spreading: Fundamental theories to cutting-edge applications. *Curr. Opin. Colloid Interface Sci.* 2018, 36, 10–19.

Extrand, C. W. A thermodynamic model for wetting free energies from contact angles. *Langmuir* 2003, 19, 646–649.

Ozdemir, O.; Karakashev, S. I.; Nguyen, A. V.; Miller, J. D. Adsorption and surface tension analysis of concentrated alkali halide brine solutions. *Miner. Eng.* 2009, 22, 263–271.

Samanta, S. K.; Bhattacharya, S.; Maiti, P. K. Coarse-grained molecular dynamics simulation of the aggregation properties of multiheaded cationic surfactants in water. *J. Phys. Chem. B* 2009, 113, 13545–13550.

Sammalkorpi, M.; Karttunen, M.; Haataja, M. Ionic Surfactant Aggregates in Saline Solutions: Sodium Dodecyl Sulfate (SDS) in the Presence of Excess Sodium Chloride (NaCl) or Calcium Chloride (CaCl2). *J. Phys. Chem. B* 2009, 113, 5863–5870.

Xi, X.; Jiang, S.; Zhang, W.; Wang, K.; Shao, H.; Wu, Z. An experimental study on the effect of ionic liquids on the structure and wetting characteristics of coal. *Fuel* 2019, 244, 176–183.