

Spreading Behavior and Wetting Characteristics of Anionic Surfactant Droplets Impacting Bituminous Coal

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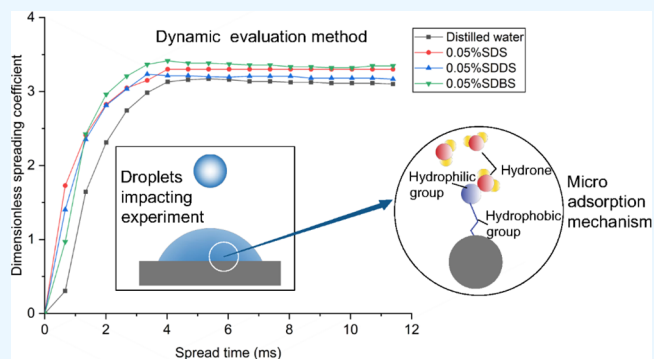
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ABSTRACT: Spraying water-based materials on the coal surface is a common means of coal dust suppression. There are obvious dynamic wetting behaviors during droplets impacting coal. To explore the spreading behavior and wetting characteristics of anionic surfactant droplets on bituminous coal, three anionic surfactants, which are sodium dodecyl sulfate (SDS), sodium dodecyl sulfonate (SDDS), and sodium dodecyl benzene sulfonate (SDBS), were used for the droplet impact experiment and molecular dynamics (MD) simulation. The results show that the addition of anionic surfactants can promote the wetting behavior of the droplet, and the difference between the head group and the tail group of the surfactant molecules can affect the wettability of the droplet. The dimensionless spreading coefficient shows the rule of SDBS > SDS > SDDS. When the concentration does not reach critical micelle concentration (CMC), the surface tension decreases and the dimensionless spreading coefficient of droplets increases with the increase of concentration. When the droplet concentration reaches the CMC, surface tension is no longer an effective indicator to evaluate the wettability of droplets. The dimensionless spreading coefficient can effectively evaluate the macroscopic spreading wetting behavior of droplets, and it is better than the surface tension. MD simulation results show that the interaction between anionic surfactants and coal molecules can affect the adsorption behavior, and the interaction energy and adhesion work are shown as the rule of SDBS < SDS < SDDS. The results of MD simulation and the impact experiment show that the intermolecular adsorption behavior has a significant influence on the spreading process. The results of MD simulation further explain the results of the droplet impact experiment.



1. INTRODUCTION

With the increasing level of coal mining mechanization, a large amount of coal dust will be generated in the production process.^{1–3} For example, the total dust concentration of the fully mechanized working face can reach 3000 mg/m³, and the respirable dust concentration usually exceeds 40% of the total dust.^{4,5} Coal dust will not only accelerate the wear and tear of equipment and reduce the service life of equipment, but also cause explosion risk and pneumoconiosis.^{6–10} Coal dust explosion is one of the most dangerous accidents in coal mines. Pneumoconiosis is the most serious occupational disease.¹¹ The United States paid more than 56.7 billion dollars to pneumoconiosis miners and their families between 2000 and 2013.¹² The number of pneumoconiosis patients in China increased by 144,000 in 2020.¹³ It can be seen that coal dust seriously affects the safe production of enterprises and threatens the health of workers.^{14–18} Spraying water-based materials on the coal surface is a frequently used method for coal dust suppression. Due to the high surface tension of water (72 mN/m), it is often ineffective in the process of wetting the coal surface. To reduce the surface tension of water and

improve its wetting efficiency, surfactants are often added to water.¹⁹

Most of the early studies showed that the wetting ability of water was significantly improved after the use of surfactants, which was conducive to improving the dust suppression effect. Fan et al.²⁰ and Xu et al.²¹ found that the addition of a surfactant to water can promote the solution properties, reduce surface tension and the contact angle of the solution, increase the wettability of the solution to coal dust, and thus improve the dust removal efficiency.²² Zhou et al.,²³ Li et al.,²⁴ and Wang et al.²⁵ studied the wetting effect of different kinds of surfactants on coal dust and found that the properties of the head groups of cationic surfactants and amphoteric surfactants are not conducive to improving the wettability of the solution

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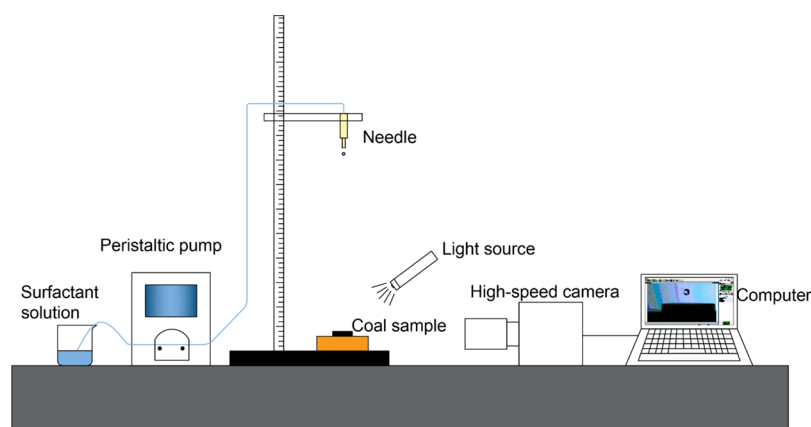


Figure 1. Experimental system of droplet impacting.

to coal dust, showing that these two kinds of surfactants are not suitable for water-based dust suppression, while anionic and nonionic surfactants can greatly improve the wetting ability of droplets to coal. Wang and co-workers²⁶ evaluated the wetting ability of three kinds of anionic surfactants on coal dust. The results showed that for the same anionic surfactant, with the increase of concentration, the adsorption density and the hydrophilic point of the coal seam surface also increased accordingly, which improved the wetting efficiency. Gui et al.²⁷ used a comparative analysis method to explore the influence factors of four surfactants on the wettability of three coal samples. The results showed that the wettability increased with the increase of the mass fraction. However, the wetting effect of the surfactant with low surface tension on coal is not necessarily good. In addition, some scholars have found that different application concentrations can be obtained by using different methods to evaluate the wetting ability of droplets.²⁸ Chen et al. found that according to the results of the sink test, the optimal concentration of SDBS for capturing coal dust was 0.2 wt %. However, for the same coal dust, the concentration was determined to be 0.3 wt % of droplet permeation experiments.²⁹ It can be seen that the existing evaluation methods have obvious deficiencies in guiding engineering practice.

Wetting coal is a process of gas substitution on the coal surface by the liquid medium. At present, the methods to evaluate the wettability of solutions are mainly to measure the surface tension of the solution or to measure the parameters in the process of slow contact between solution and coal such as the surface tension experiment, contact angle experiment, sink test, capillary rise experiment, and droplet penetration experiment.^{30–38} Although the contact angle can reflect the wetting relationship between surfactant solution and coal, the surface of coal is required to be smooth. Otherwise, the measurement results often show obvious error.³⁹ In addition, although it is convenient to use the contact angle or its derivative quasi-static wetting index to evaluate the dust control ability of droplets, it still has obvious optimization space because it does not consider the dynamic effect in the actual dust control process.⁴⁰ Droplets often cannot wet coal surfaces effectively. Sometimes they bounce and slide, or coalesce and lost, which not only wastes water resources, but also affects the environment of the workplace. The sink test cannot accurately evaluate the wetting ability of the solution at a low concentration. Moreover, the dynamic wetting characteristics of the droplet wetting process were not considered in the

sink test and capillary rise experiment. In the practice of coal dust prevention and control, the droplets are moving, and there will be spread, splash, and other phenomena when the droplets hit the coal surface, which shows obvious dynamic characteristics. Dynamic wetting characteristics of droplets on the coal surface directly affect its utilization rate and dust control efficiency, which is of great significance to dust control practice.

In the field of coal dust control, anionic surfactants sodium dodecyl sulfate (SDS), sodium dodecyl sulfonate (SDDS), and sodium dodecyl benzene sulfonate (SDBS) are widely used.^{41–43} Therefore, in this paper, the impact of dust suppression droplets on the coal surface was studied. The mentioned three kinds of anionic surfactants were selected to conduct droplet impact experiments on the coal surface. The impact behavior and wetting characteristics at different concentrations were analyzed. The molecular dynamics (MD) simulation method was used to study the interaction between anionic surfactants and coal molecules. The research results are of great significance for optimizing the evaluation method of droplet wetting ability and selecting economic and efficient dust suppressants.

2. EXPERIMENT AND METHOD

2.1. Materials. The coal samples involved in this experiment are from Wangzhuang Coal Mine, Luan Group. The entire sampling process was strictly conducted as described by national guidelines (GB475-2008). The coal samples were crushed by a coal crusher, and then 40~60 mesh pulverized coal with particle size distribution of 250~380 μm was obtained by standard screening. Using the YP-40T desktop powder tablet press from Tianjin Jifulun Technology Co., Ltd., the quantitative pulverized coal was pressed into cylindrical thin slices with a diameter of 20 mm and a height of 5 mm under a working pressure of 20 MPa.

The working fluids used in this experiment were distilled water, SDS (analytically pure), SDDS (analytically pure), and SDBS (analytically pure). Surfactants were configured at 0.01, 0.05, and 0.1 wt % respectively. Distilled water is used to prepare all solutions.

2.2. Experimental Systems for Droplet Impact. The droplet impact experiment system mainly includes a droplet generator (composed of a peristaltic pump, silicone tubes, a needle tube joint, etc.), an adjusting bracket, background light sources, a high-speed camera (VEO-340), and an image acquisition computer, as shown in Figure 1. In this experiment,

the frame number of the high-speed camera is 1500 f/s, and the pixel is 1920 pixel \times 1080 pixel. The experimental device is illuminated by a cold light source to ensure that the image is clear. The captured images are recorded by a computer in real time. The initial velocity of the droplet is 1.5 m/s. The experiment was carried out at room temperature, and the coal surface was kept dry. To reduce the influence of surface humidity on the impact process, the surface was washed with hot water before each experiment, dried at 80 °C for 0.5 h, and then cooled to room temperature in cold air. The relative humidity of the room during cooling is 45%. The images obtained in the experiment were processed by the Phantom Camera Control Software.

In the experiment of droplets impacting the coal surface, the spreading length is an important parameter to show the spreading degree. Therefore, in this paper, the initial diameter of the droplet is defined as d_0 . The spreading length of the droplet on the solid plane is defined as d , and the maximum spreading length is d_{\max} . Then, the dimensionless spreading coefficient is $\beta = d/d_0$, and the maximum dimensionless spreading coefficient is $\beta_{\max} = d_{\max}/d_0$. The influence of different droplets on the impact coal surface was explored by recording the spreading behavior of different droplets and the change of the dimensionless spreading coefficient during the experiment.

2.3. Surface Tension Test. The JK99D automatic surface tension meter from Shanghai Zhongchen Digital Technology Equipment Co., Ltd. was selected to measure the surface tension of the above nine solutions and distilled water at room temperature. The test method is the hanging plate method, that is, slowly moving the platform during the test and gently contacting the platinum plate to the liquid surface until it immersed in the liquid (the size of the platinum plate is 24 mm \times 10 mm \times 0.1 mm, and its surface has been coarsened by sandblasting). In the immersion state, the balance value is detected by the inductor. After the data displayed by the computer are stabilized, a reading can be performed to complete a measurement. Before each measurement, the platinum plate was cleaned with distilled water and then dried on the alcohol lamp. Distilled water was used for data verification.

The average surface tension value was obtained by three measurements of each solution, and the difference between the three test results was within 0.2 mN/m.

2.4. Viscosity Test. The NDJ-5S rotary viscometer from Shanghai Pinguan Scientific Instrument Co., Ltd. was used to measure the viscosity of the distilled water and solution. The selected No.1 rotor is mounted on the instrument, and it is immersed in the liquid to be measured until the liquid surface is equal to the sign on the rotor. After setting the parameters such as speed, the measurement begins, and the solution temperature needs to be accurately controlled. Each result is the average of three measurements.

2.5. MD Simulation. To reveal the interaction between anionic surfactant molecules and coal molecules, the interaction energy and adhesion work of anionic surfactant molecules and coal molecules were calculated by Material Studio 2019. The coal-anionic surfactant-water model was constructed in Forcite module. The model is composed of geometrically optimized coal molecules, anionic surfactant molecules, and water molecules. The charge of the molecule is automatically assigned by the COMPASS II force field. As shown in Figure 2a, the bituminous coal surface model consists

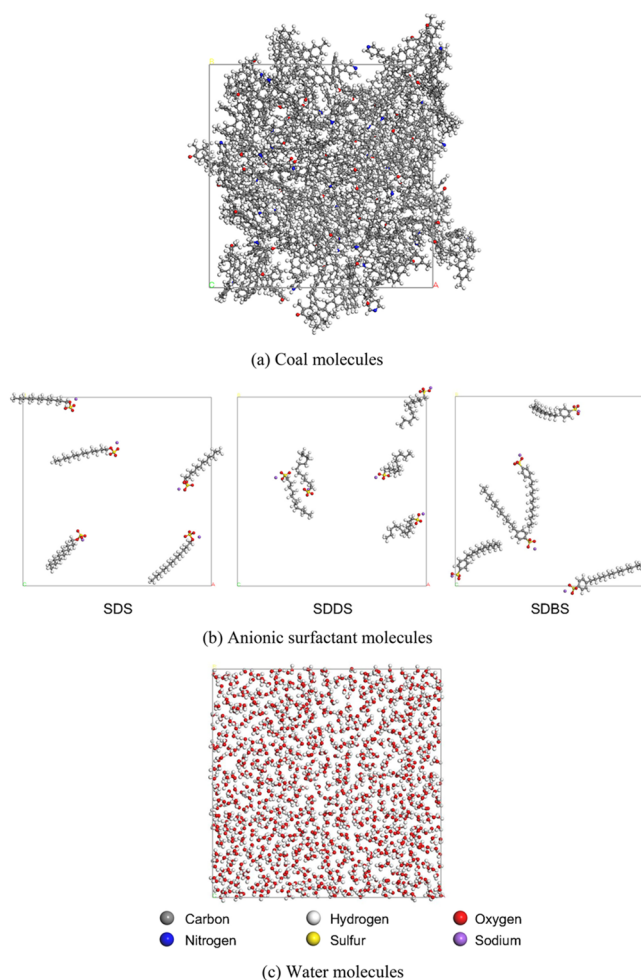


Figure 2. Models of individual components. (a) Coal molecules. (b) Anionic surfactant molecules. (c) Water molecules.

of 20 geometrically optimized bituminous coal molecules which filled into a 3D cell of size 50 Å \times 50 Å \times 18.8 Å ($X \times Y \times Z$). As shown in Figure 2b,c, the cells of anionic surfactant consist of five SDS, SDDS and SDBS molecules, respectively, and the cell of water molecule contains 1000 water molecules.

The Layer Builder program was used to combine coal, anionic surfactant, and water molecules, as shown in Figure 3a. The established coal-anionic surfactant-water model was optimized geometrically to make it closer to the real molecular

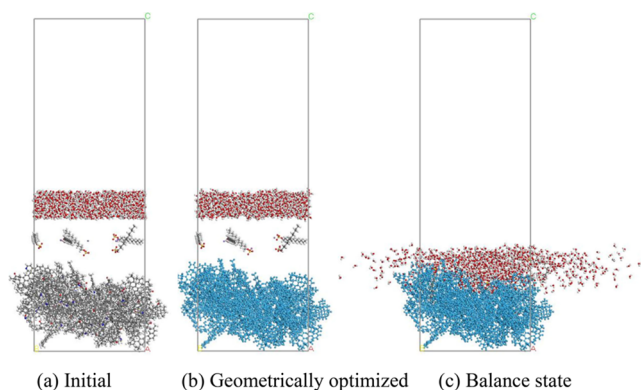


Figure 3. Interface model. (a) Initial, (b) geometrically optimized, and (c) balance state.

structure. The optimized coal-anionic surfactant-water model is shown in Figure 3b. Subsequently, it runs under the NVT ensemble at 298 K. The target temperature and pressure in the system are maintained by using the Nose thermostat and the Andersen, and the time step is set to 1.0 fs. The cutoff value of van der Waals interaction is 15.5 Å, and the long-range electrostatic interaction is explained by the Ewald summation method (the accuracy is 10^{-3} kcal/mol). In the process of MD simulation, the coal surface is frozen. Related studies have shown that the constraints on coal surface molecules have little effect on the calculation results.⁴⁴ The results are calculated based on the simulation results lasting 200 ps after the equilibrium period. The equilibrium state after the simulation is shown in Figure 3c.

3. RESULTS AND DISCUSSION

3.1. Effect of Anionic Surfactants on Droplet Spreading Behavior. Three kinds of anionic surfactants and distilled water droplets hit the coal surface at a speed of 1.5 m/s. Different types of droplets show different spreading behaviors. It can be observed from Figure 4 that after the distilled water

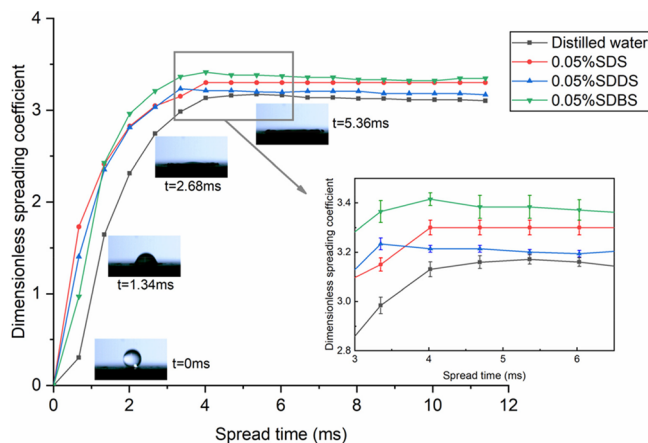


Figure 4. Different droplets' spreading behaviors.

droplets hit the coal surface, the droplets spread rapidly due to the initial kinetic energy. The edge of the droplet gradually transits from a sharp spine shape to a semicircular shape, and the droplet is a pagoda shape ($t = 1.34$ ms). After that, the droplets continue to spread symmetrically along the horizontal direction and the height of the droplet center gradually decreased. When the droplet reaches the maximum spreading, the droplet shows an approximately round cake ($t = 5.36$ ms). At this time, the maximum dimensionless spreading coefficient β_{\max} is 3.17. Finally, the droplet retracts under the action of surface tension and oscillates violently up and down until it reaches equilibrium. In this process, the initial kinetic energy gradually transforms into viscous dissipation and friction dissipation. The spreading phenomenon of 0.05 wt % SDS, 0.05 wt % SDDS, and 0.05 wt % SDBS droplets is similar to that of distilled water droplets. However, the time to reach the maximum spreading diameter of the three droplets is 4.02, 3.35, and 4.02 ms respectively, which are less than 5.36 ms of distilled water droplets. The maximum dimensionless spreading coefficient β_{\max} is 3.30, 3.23, and 3.42, respectively.

It can be seen that the spreading behavior of surfactant droplets is better than that of distilled water droplets during the process of droplets hitting the coal surface from the

experimental data. Droplets containing surfactants can spread rapidly and exhibit better wettability after coming in contact with the coal surface. The reason is that there is a strong interaction between the surfactant molecules and the hydrophobic groups on the coal surface. The hydrophobic tail of the surfactant molecules is adsorbed on the hydrophobic water level point of the coal surface, forming a directional adsorption layer of hydrophobic groups toward coal and hydrophilic groups toward water molecules. Meanwhile, surfactant molecules are equivalent to bridges connecting coal molecules and water molecules as shown in Figure 5. In this process, the

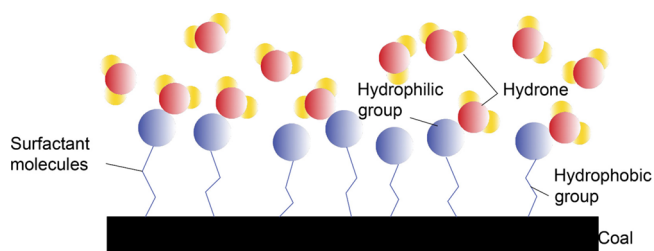


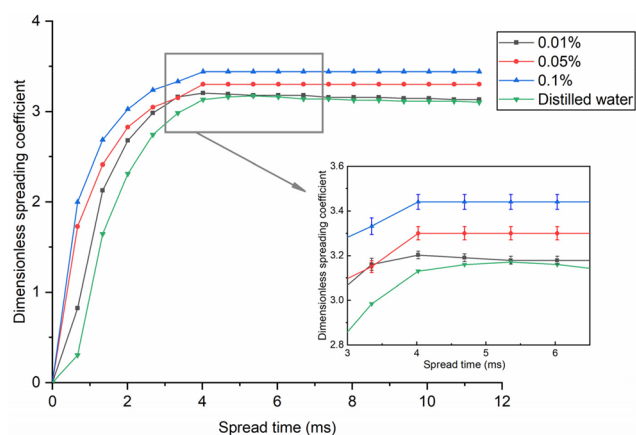
Figure 5. Wetting mechanism of surfactant molecules.

hydrophilic and hydrophobic groups of surfactant molecules will quickly aggregate on the surface of the solution due to the attraction and repulsion of water molecules, thus making the surface tension of the solution less than the critical surface tension (45 mN/m) and promoting the wetting behavior.

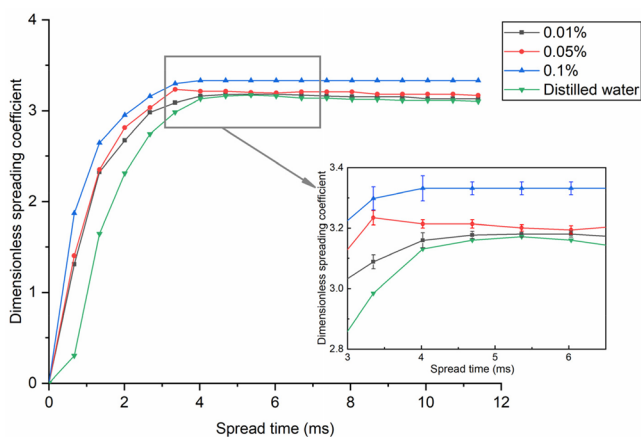
In addition, at the same concentration, the dimensionless spreading coefficient of the solution always follows the rule of SDBS > SDS > SDDS. The hydrophobic group of SDS and SDDS is alkyl, and the hydrophilic group is the sulfate group and sulfonate group, respectively. The hydrophobic group of SDBS is alkyl benzene, and the hydrophilic group is the sulfonate group. Compared with SDS and SDDS, SDBS showed strong wetting ability. The reason is that SDBS has the longest tail group and the highest adsorption density of hydrophobic groups, which could produce more hydrophilic water points on the surface of the coal. Although SDS and SDDS have the same tail group, the head group structures are different. The sulfate group is more hydrophilic than the sulfonate group. Therefore, at the same concentration, SDS has a larger dimensionless spread coefficient than SDDS, and the wetting effect is better.

In summary, the spreading behavior of droplets with the anionic surfactant in the process of impacting the coal surface is more rapid and stable than that of distilled water. The time to reach the maximum spreading diameter is shorter than that of distilled water, and the maximum dimensionless spreading coefficient is greater than that of distilled water droplets. This phenomenon explains that adding an anionic surfactant in dust control practice can increase the efficiency of droplet spreading and wetting. However, the effects of different surfactant structures on droplet impact behavior are significantly different.

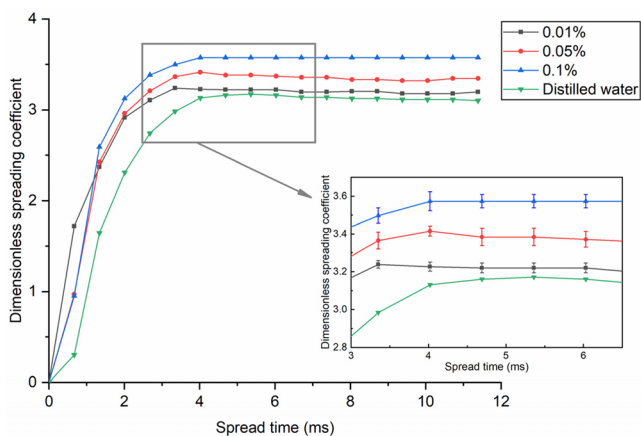
3.2. Effect of Surfactant Concentration on Droplet Spreading Behavior. The dynamic wetting behaviors of the same anionic surfactant at different concentrations are not the same. The spreading behavior curves of three kinds of anionic surfactants are obtained by the impact experiment. As shown in Figure 6a, when the concentration of SDS solution is 0.01 wt %, the droplet reached the maximum spreading diameter and then retracted, while when the concentration was 0.05 and 0.1



(a) Spreading behaviors of SDS droplets impacting on coal surface



(b) Spreading behaviors of SDDS droplets impacting on coal surface

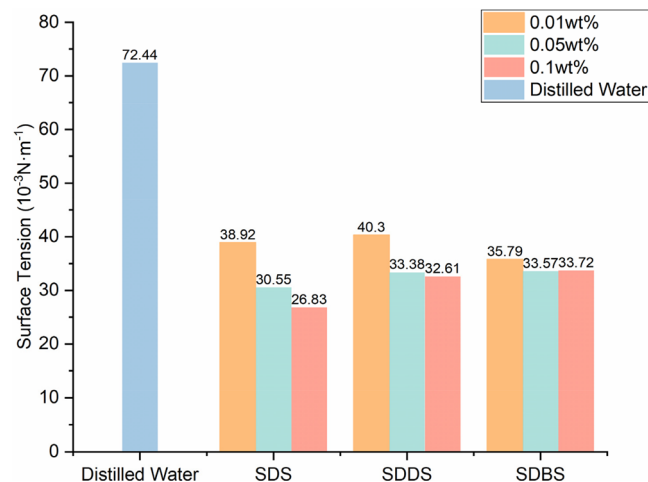


(c) Spreading behaviors of SDBS droplets impacting on coal surface

Figure 6. Spreading behaviors of droplets with different concentrations. (a) Spreading behaviors of SDS droplets impacting on the coal surface. (b) Spreading behaviors of SDDS droplets impacting on the coal surface. (c) Spreading behaviors of SDBS droplets impacting on the coal surface.

wt %, no retraction occurred. **Figure 6b,c** shows that the SDDS solution retracted when the concentration is 0.01 and 0.05 wt % and does not retract when the concentration is 0.1 wt %. The spreading behaviors of SDBS droplets are the same as those of SDDS. The reason for the phenomenon may be that the surface tension of the solution decreases with the increase of the concentration. Droplets always have a tendency to

reduce the surface free energy. When the surface tension is constant, reducing the surface area of droplets is the only way to reduce the surface free energy, so the spreading droplets always have a tendency to retract. **Figure 7** shows the surface

**Figure 7.** Surface tension histograms of different droplets.

tension values of different solutions. Surface tension is the driving force to control the droplet retraction during the spreading process. When the surface tension is less than a certain value, it is not enough to overcome the viscous dissipation of the droplet and thus the retraction no longer appears. For example, the surface tension of the SDDS solution at 0.1 wt % is 32.61 mN/m, which is the smallest of the three concentrations. The energy to promote retraction is not enough to overcome the viscous dissipation, so the retraction does not occur.

It can be seen from the above examples that the viscosity of the droplet also affects the spreading behavior to a certain extent. In the process of droplet spreading, the viscous dissipation of droplets with high viscosity is large, which is not conducive to the spreading of droplets. The viscous force inhibits the retraction of the droplets during retraction. The surface tension of SDBS solution is almost the same when the concentration is 0.1 and 0.05 wt %. However, the retraction phenomenon occurs when the concentration of SDBS solution is 0.05 wt % and does not retract when the concentration is 0.1 wt %. The reason may be that the viscosity of 0.05 wt % solution is small. Thus, the surface tension can overcome the viscous force. The viscosity of 0.1 wt % solution and the viscous force is larger, and the surface tension is not enough to overcome the viscous force. Thus, it does not retract.

In summary, no matter what kind of solution, the dimensionless spreading coefficient of droplets gradually increases with the increase of surfactant concentration. This is because as the concentration increases, the surfactant molecules are more likely to spontaneously adsorb on the surface layer of the solution, so that the surface tension of the droplets decreases. In most cases, droplets with small surface tension can achieve a better spreading effect. However, **Figure 7** shows that the values of surface tension of the SDBS solution at 0.05 and 0.1 wt % are approximately equal (33.57 and 33.72 mN/m), and the maximum dimensionless spreading coefficient at 0.1 wt % is larger than that at 0.05 wt % (3.57 > 3.42). In the anionic surfactant solution system, with the increase of concentration, the adsorbed surfactant molecules at

the gas–liquid interface gradually reach saturation. When the concentration increases again and reaches the critical micelle concentration (CMC), surfactants in the aqueous phase began to form a large number of micelles in the form of hydrophobic chain facing inward, and the surface tension of the solution will not continue to decrease. For SDBS solution, 0.05 and 0.1 wt % have exceeded the CMC value (0.04 wt %), which is the main reason why the values of surface tension of SDBS solution do not change significantly under these two concentrations. When the SDBS solution reaches the CMC value, the adsorption density of the coal surface increases with the increase of the concentration. As described in Section 3.1, more hydrophobic water points on the coal surface are converted into hydrophilic water points, so that the wetting behavior of the droplet is better. In addition, compared with distilled water, the surface tension of the surfactant-added droplets decreased significantly, while the spreading behavior of the droplets did not change significantly. This is because during the impact experiment, the wetting of droplets on the coal surface is a complex process involving many factors. The wettability of droplets on coal dust is affected by the type, concentration, impact velocity of droplets, physical and chemical properties of coal surface, and the interaction between droplets and coal. Therefore, the surface tension is not the decisive index to evaluate the spreading behavior of dynamic droplets impacting on solid surface, and this parameter has certain limitations. This reflects the scientific and accuracy of using the method of impact experiment to evaluate the spreading behavior of droplets on coal surface by dimensionless spreading coefficient. This parameter can more effectively guide the selection of surfactants in engineering practice.

3.3. Interaction between Anionic Surfactant Molecules and Coal Molecules. To further study the wetting mechanism of anionic surfactants, the MD simulation method is used to analyze the interaction between anionic surfactants and coal molecules. Simulation results show that the coal-anionic surfactant-water system mainly reaches the thermodynamic equilibrium state driven by nonbond interactions such as van der Waals interaction and electrostatic interaction. The energy calculation results are shown in Figure 8. It can be seen that the absolute value of van der Waals interaction energy (EV) in the system is much larger than that of electrostatic interaction energy (EL), indicating that the adsorption is mainly caused by van der Waals interaction energy. This is

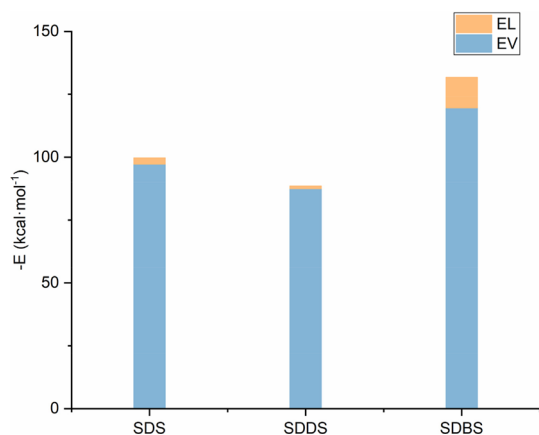


Figure 8. Calculation results of nonbond interaction energy.

because the three surfactants are all anionic surfactants. The surfactant ions are negatively charged, and the oxygen-containing functional groups of coal molecules are less and negatively charged. The electrostatic interaction between them is minimal.

The calculation results show that the van der Waals interaction energy of the SDBS system is stronger than that of SDS and SDDS. The adsorption caused by van der Waals interaction energy between coal and surfactant molecules increases with the increase of molecular weight. The presence of the benzene ring in SDBS increases the molecular weight and makes the adsorption configuration more stable. SDS molecules have one more oxygen atom than SDDS molecules, which increases their molecular weight. Thus van der Waals interaction is stronger than SDDS. In addition, there is a strong pi-pi stacking effect between the benzene ring structure in SDBS molecules and the aromatic structure of the coal molecule,^{45,46} which may also be the reason for the more stable adsorption of SDBS.

In addition, using adhesion work to evaluate the adsorption behavior between surfactants and coal molecules is helpful to understand the interaction between them. Adhesion work (W_{adhesion}) is the work done by separating surfactant from coal at the interface. The adhesion work is calculated by Formula 1, and the interaction energy (E_{inter}) is calculated by Formula 2.

$$W_{\text{adhesion}} = E_{\text{inter}}/A \quad (1)$$

$$E_{\text{inter}} = E_{\text{total}} - (E_{\text{coal}} + E_{\text{surfactant}}) \quad (2)$$

W_{adhesion} is the interfacial adhesion work. E_{inter} is the interaction energy of the system. E_{total} is the total potential energy of coal and surfactant molecules when the system is stable. E_{coal} and $E_{\text{surfactant}}$ are the potential energy of coal and surfactant respectively. A is the contact area of the two. The interaction energy can represent the interaction strength between coal and surfactant. When the interaction energy (E_{inter}) and adhesion work (W_{adhesion}) are negative, the adsorption process between the surfactant and coal is spontaneous, and the adsorption intensity increases with the decrease of interaction energy and adhesion work. The results of interaction energy and adhesion work of three surfactants are shown in Table 1.

Table 1. Energy between Three Surfactants and Coal Molecules

	E_{inter} (kcal mol ⁻¹)	W_{adhesion} (mJ m ⁻²)
SDS	-101.23	-28.16
SDDS	-90.02	-25.04
SDBS	-133.75	-37.20

From the above results, it can be seen that the interaction energy and the adhesion work of the three surfactant systems are negative. The interaction energy and the adhesion work of the SDBS system are the smallest while those of the SDDS system are the largest. This indicated that the adsorption strength between SDBS and coal molecules is the highest, and the formed adsorption system is more stable than the other two surfactants, followed by SDS, and SDDS has the weakest adsorption capacity. Macroscopically, the adsorption ability of surfactant molecules on the coal surface is the ability of the surfactant to change the wetting ability of a solution. When the interaction is strong, the droplet wetting ability is strong and the spreading effect is better. Therefore, the simulation results

show that the interaction between SDBS molecules and coal molecules is the strongest. According to the experimental results, the dimensionless spreading coefficient of SDBS solution in these three anionic surfactants is the largest. The simulation results further prove the reliability of the experiment.

4. CONCLUSIONS

In this paper, three kinds of anionic surfactants are used to carry out droplet impact experiments. The effects of the physical properties and concentration of the droplet on the dynamic wettability of the droplet are investigated. The main conclusions are as follows:

- (1) During impacting on the coal surface, the spreading behavior of droplets containing anionic surfactants is better than that of distilled water droplets, indicating that the addition of anionic surfactants improves the dynamic wettability of droplets. At the same concentration, the rule of the maximum dimensionless spreading coefficients of the three anionic surfactant solutions always shows SDBS > SDS > SDDS. The droplet spreading behavior is related to the structure of the surfactant molecules. The long-chain tail group makes the adsorption density higher, and the head group structure can lead to different hydrophilicity.
- (2) When the surfactant concentrations do not reach the CMC value, the maximum dimensionless spreading coefficient of droplets increases with the increase of concentrations. When the solution concentrations reach the CMC value, surface tension is not a decisive indicator for evaluating droplet spreading behavior. Surface tension and viscosity jointly affect the spreading behavior and wetting characteristics of droplets. At this time, the dimensionless spreading coefficient is a more effective in evaluating indicator.
- (3) The adhesion of the anionic surfactant to the coal surface is spontaneous, and the adsorption behavior is mainly caused by van der Waals interaction. The larger the molecular weight is, the stronger the adsorption is. The macroscopic performance of adsorption is the wettability of droplets, and the results of MD simulation proved the reliability of the experimental results.

■ CONSENT TO PUBLISH

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Notes

The authors declare no competing financial interest.

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■ ABBREVIATIONS

SDS	sodium dodecyl sulfate
SDDS	sodium dodecyl sulfonate
SDBS	sodium dodecyl benzene sulfonate
CMC	critical micelle concentration
MD simulation	molecular dynamics simulation

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