Experimental and Molecular Dynamics Simulation Study for Preferring Coal Dust Wetting Agents

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ABSTRACT: To improve the efficiency of coal dust removal by water spray technology, the addition of wetting agents in water becomes the main dust removal method. The influence of sodium dodecyl sulfate (SDS), sodium dodecyl sulfonate (SDDS), and sodium dodecylbenzene sulfonate (SDBS) on the wettability of coal dust is studied by experimental and molecular dynamics (MD) simulation. Measurement of the contact angle and surface tension was accomplished via relevant experiments for the three wetting agents, and their adhesion work, spreading work, and wetting work were also calculated. A preferred experimental method of conventional coal dust wetting agent is optimized. The wettability of the three wetting agents upon bituminous coal follows the trend: SDS > SDDS > SDBS. The simulation was performed based on MD to derive the intermolecular interaction energy, diffusion coefficient of water molecules, and water molecule count in the vicinity of the hydrophilic groups of the wetting agents. The wetting mechanism and performance of the wetting agent solution on bituminous coal were identified. The simulation results of the wetting performance of the wetting agents are consistent with the experimental results, which verifies the reliability of the simulation method. An easy, time-saving, and labor-saving MD simulation method is proposed, which provides a novel insight for choosing various wetting agents of coal dust.

1. INTRODUCTION

During manufacturing and transportation of coal from mines, massive coal dust is produced, which causes pneumoconiosis in coal miners.1−3 Pneumoconiosis is a preventable but incurable lung disease, which not only causes chest pain but also causes significant complications such as chronic cor pulmonale and respiratory failure.4−6 Nowadays, the main dust removal method used in coal mines is spray dust removal.7−9 Water is ineffective in wetting coal dust since its surface tension reaches 72.8 mN/m, while for coal, it is 45 mN/m at critical wetting.10,11 To lower the surface tension and enhance the wettability of coal, wetting agents can be incorporated into water.12−14

So far, many researchers have studied the influence of various wetting agents on the wettability of coal through static experiments.15 Yan et al.16 used a contact angle measuring instrument to determine the wettability of different compound surfactants. Then, the preferred surfactants were compounded with chemically modified sodium alginate to prepare an environmentally friendly coal dust wetting agent. Sun et al.17 used starch as a raw material and modified it by adding methyl methacrylate and an acrylamide monomer. Then, hexadecyl trimethyl ammonium bromide was added for compounding. The wettability of coal dust was determined by the contact angle parameter, and the wettability mechanism of the dust suppressant to coal dust was revealed by Fourier-transform infrared spectroscopy, X-ray diffraction, and scanning electron microscopy instruments. Jiang et al.18 studied the effects of surfactant type, mass fraction, coal deterioration degree, particle size, and additives on the wettability of coal dust by contact angle parameters, and the optimal surfactant was selected. The above research studies only determine the wettability of different surfactants to coal dust by the contact angle parameter, and the surface tension of the wetting agent also affects the wettability of coal dust. According to the
The wetting process of coal dust, the wettability of different surfactants on coal dust was studied by introducing three parameters: adhesion work, spreading work, and wetting work. To master the wettability of different wetting agents on coal dust from a microaspect, an easy, time-and-labor-saving molecular dynamics (MD) simulation method is proposed. According to the surfactant adsorption process, mainly studying the wettability of single surfactants on coal dust. Niu et al.19 took APG-12 as the research object and revealed the mechanism of APG-12, improving the wettability of coal dust by analyzing the electrostatic potential, surface static charge distribution, and relative concentration distribution. Yuan et al.20 studied the adsorption process of AEO-9 solution on a lignite surface by the MD simulation method. According to the surfactant adsorption structure, concentration distribution curve, water molecular diffusion coefficient, and interaction energy, AEO-9 has good wettability to lignite. Liu et al.21 studied the effect of sodium fatty alcohol polyoxyethylene ether carboxylate (AEC) on the wettability of lignite through structural features of the simulation systems, interaction energy, and water molecular diffusion coefficient. The simulation results show that AEC enhances the interaction of coal–water. Compared with traditional experiments, it has the advantages of a short research cycle and low cost.

In this paper, the effects of three anionic wetting agents, sodium dodecyl sulfate (SDS), sodium dodecyl sulfonate (SDDS), and sodium dodecylbenzene sulfonate (SDBS), upon the wettability of bituminous coal were discussed by employing both experimental and simulation methods. The study improves the preferred experimental methods of coal dust wetting agents and proposes a preferred MD simulation method of coal dust wetting agents and reveals the wetting mechanism of the wetting agent solution to coal dust.

2. EXPERIMENT AND SIMULATION

2.1. Materials. Bituminous coal from the Xindingtai coal mine in Lingshi County, Jinzhong City, China, was taken as the research object for the study. Table 1 details the elemental analysis result of the coal specimen, whose size was ≤74 μm by ball milling and vibrating screen. The prepared coal specimen was subjected to 24 h of vacuum drying in an oven set at 40 °C and then transferred into a dryer for later experimental use. SDS and SDDS used in the experiment were provided by Tianjin Zhiyuan Chemical Reagent Co., Ltd., and SDDS was provided by Fuzhou Feijian Biotechnology Co., Ltd.

2.2. Experimental Process. The mass concentrations of the wetting agents were 0.01, 0.03, 0.05, 0.07, 0.09, 0.1, 0.3, and 0.5% in tap water. An SDC-350 contact angle measuring apparatus (Shengding Precision Instrument, Dongguan) was employed to measure the contact angle and surface tension. The measurement methods were the hanging drop method and angle measurement method, with an accuracy of 0.01 mN/m and ±1°, respectively. The coal pellets in the contact angle were prepared using a tablet press; the mass was 50 mg, the pressure was 20 MPa, and the time was 2 min. Each group experiment was carried out three times.

2.3. Simulation Details. Coal is a macromolecule with a complex structure, which is mainly composed of organic and inorganic compounds. As for the molecular structure of coal, the current technology cannot accurately determine the molecular model of actual coal. Li,22 Zhang,23 Yuan,20 and Niu et al. used classical lignite and sub-bituminous coal models instead of experimental coal models to conduct MD simulation studies. Because coal in the experiment is bituminous coal,24 the more comprehensive and reasonable Wisser’s bituminous coal model is selected for MD simulation. The density and porosity of the coal are 1.27 g/cm and 4.87%, respectively. The molecular structures of bituminous coal (C_{19}, H_{166} N_{3} O_{21} S_{3}), SDS (C_{12} H_{24} S O_{4} Na), SDDS (C_{12} H_{25} S O_{4} Na), and SDBS (C_{18} H_{39} S O_{4} Na) are depicted, respectively, in Figure 1a–d.

All molecular calculations were performed using the Compass II forcefield.25–27 The forcefield has broad coverage in covalent molecules including most common organics, small inorganic molecules, and polymers. The combination of parameters for organics and inorganics makes the study of interfacial and mixed systems possible. Therefore, the Compass II forcefield is suitable for H$_2$O–wetting agent–bituminous coal systems. The molecular simulation steps are shown in Table 2.

The geometry optimization was used to optimize the bond length and bond angle of molecules, and the related parameters were as follows: the algorithm was smart; the maximum iterations were 50,000; the maximum convergence values of energy, force, displacement, and maximum iteration were 1.0 $\times$ 10$^{-4}$ kcal/mol, 5 $\times$ 10$^{-3}$ kcal/mol Å, and 5 $\times$ 10$^{-5}$ Å, respectively. To compare the wetting performance of different wetting agents, the mass concentration of wetting agents should be the same. The number of molecules corresponding to SDS, SDDS, and SDBS was 18, 19, and 20. The annealing method was used to further optimize the bond length, bond angle, and conformation of the molecules; the initial temperature and midcycle temperature were 298 and 1098 K, respectively. The related parameters of MD simulation were as follows: the ensemble was NVT (N: the number of particles is conserved, T: constant temperature, V: constant volume), and the temperature was 298 K. The temperature control method was NHL (Nose–Hoover–Langevin dynamics is a method for performing constant-temperature dynamics that produces true canonical ensembles in both coordinate space and momentum space); it is suitable for the isothermal ensemble. The step size was set as 1 fs, and the total time was 17593
2000 ps. At 2000 ps, the energy and temperature of systems tend to stabilize, indicating that the systems reach balance. The Ewald summation technique with high precision was used for computing the electrostatic interaction and the van der Waals interaction. The related parameters were as follows. The summation accuracy and the repulsive cutoff of electrostatic interaction energy were 0.001 kcal/mol and 0.5 Å, respectively. The summation accuracy, the repulsive cutoff, and buffer width of van der Waals energy were 0.001 kcal/mol, 12 Å, and 0.5 Å, respectively.

3. RESULTS AND DISCUSSION

3.1. Experimental Results. 3.1.1. Evaluation Parameters of Bituminous Coal Wettability. There are mainly two parameters that can be used to access the wettability of wetting agents: contact angle and surface tension. The lower the surface tension, the easier the droplets are to break and the larger the contact area between coal dust and droplets, and accordingly, the wettability is improved. The smaller the contact angle, the easier will be the immersion of the droplets in coal and hence better the wetting effect. Figures 3 and 4, respectively, show the surface tension variations and contact angle variations against concentration for various wetting agents. Figure 3 suggests that the surface tension of SDDS is the highest. According to Figure 4, SDBS exhibits the largest contact angle. The wettability of wetting agents obtained by surface tension and contact angle measurements is inconsistent, so adhesion work, spreading work, and immersion work are introduced to characterize the wettability of the wetting agent.

3.1.2. Process of Wetting Bituminous Coal with the Wetting Agent Solution. The wetting process of coal dust with the wetting agent solution mainly includes three parts: adhesion, spreading, and immersion, as shown in Figure 5. Adhesion is defined as a progressive replacement process of the gas−liquid and gas−solid interfaces by the solid−liquid interface. Spreading refers to the phenomenon where the solid−liquid adhesion is greater than or equal to the cohesion work of a liquid. Immersion refers to the wetting process of a
solid immersed in a liquid. The greater the wetting work, spreading work, and immersion work, the better the wetting performance of bituminous coal. The calculation formulas are shown in 1−3, respectively.

\[ W_a = \gamma (1 + \cos \theta) \]  
\[ S = \gamma (\cos \theta - 1) \]  
\[ W_i = \gamma \cos \theta \]  

where \( W_a \) is the adhesion work, mN/m; \( \gamma \) is the surface tension, mN/m; \( \theta \) is the contact angle, °; \( S \) is the spreading work, mN/m; and \( W_i \) is the immersion work, mN/m.

Figures 6–8 show the adhesion work, spreading work, and immersion work of the three wetting agents at different concentrations, respectively. The variations of these three parameters with concentration follow the same trend: SDS > SDDS > SDBS; that is, the results are consistent. Therefore, the wettability of the three wetting agents for bituminous coal is SDS > SDDS > SDBS.

3.2. Simulation Results. 3.2.1. Interaction Energy. The molecular interaction energy can represent the strength of the intermolecular interaction. The lower its value, the stronger will be the intermolecular interaction. When the mass concentrations of the wetting agents were the same in simulation systems, the lower the interaction energy between wetting agents and bituminous coal, the better the wetting properties of bituminous coal.20 The molecular potential energy can be used to characterize the molecular interaction energy (\( E_{\text{interaction}} \)) of each system; the calculation formula is

\[ E_{\text{interaction}} = E_{\text{total}} - (E_{\text{H}_2\text{O} - \text{wetting agent}} + E_{\text{bituminous coal}}) \]  

where \( E_{\text{total}} \) is the potential energy of the water−wetting agent−bituminous coal system; \( E_{\text{H}_2\text{O} - \text{wetting agent}} \) is the potential energy without bituminous coal; and \( E_{\text{bituminous coal}} \) is the potential energy of bituminous coal.

Table 3 is the interaction energy of different systems. The main interaction energies between molecules are electrostatic energy and van der Waals energy, and electrostatic energy plays a major role. The wetting performance of different solutions to bituminous coal follows the trend SDS > SDDS > SDBS > H₂O. When wetting agents are not added to the water, the interaction energy between water molecules is −23,874.27 kcal/mol. After the addition of SDS, SDDS, and SDBS in water, the interaction energy between the water molecules is reduced to −20,247.16, −20,523.54, and −21,974.02 kcal/mol, resulting in a decrease in cohesion between water molecules. The interaction energy between water molecules is larger, and the cohesion is smaller, resulting in a stronger interaction...
between the wetting agent solution and bituminous coal, and the wetting effect of bituminous coal is better.

### 3.2.2. Mean Square Displacement

The addition of wetting agents to water will affect the movement of water molecules. The diffusion capability of water molecules can be determined by comparing and analyzing the mean square displacement (MSD) curve and diffusion coefficient D of water molecules in the system before and after the addition of wetting agents. The MSD is calculated as follows:

$$\text{MSD}(t) = \frac{1}{N} \lim_{t \to \infty} \frac{d}{dt} \sum_{i=1}^{N} \langle [r_i(t) - r_i(0)]^2 \rangle$$

where N is the number of water molecules in the system, \(r_i(0)\) is the position of water molecules at \(t = 0\), and \(r_i(t)\) is the position of water molecules at the instant \(t\). D is calculated as follows:

$$D = \frac{1}{6} \lim_{\Delta t \to \infty} \frac{\text{dMSD}}{\text{d}t}$$

Figure 9 is the curve of the MSD (Å²) analysis. In SDS, SDDS, SDBS, and water solutions, the diffusion coefficients of water molecules are 5.559 × 10⁻⁹, 5.673 × 10⁻⁹, 5.982 × 10⁻⁹, and 6.783 × 10⁻⁹ m²/s, respectively. After wetting agents are added to the water, the wetting agent hydrophobic groups are adsorbed on the surface of the bituminous coal, and the hydrophilic groups are adsorbed on the water surface, as shown in Figure 10 (taking 18 SDS as an example). The surface of the bituminous coal is covered by the hydrophilic groups of the wetting agents, and water molecules are attracted by the oxygen atoms in the hydrophilic groups under the action of electrostatic force and hydrogen bonds. As a result, the diffusion ability of water molecules decreases, the number of water molecules on the surface of bituminous coal increases, and the wettablility is enhanced. The smaller the diffusion coefficient of water molecules, the better the wetting effect of bituminous coal.

### 3.2.3. Radial Distribution Function

To determine the water molecule count on the surface of the bituminous coal, radial distribution function (RDF) analysis was proposed. The RDF represents the probability of one atom appearing at some distance from another atom and is calculated according to eq 7.

$$g(r) = \frac{dN/(4\pi r^2 \, dr)}{N/(a \times b \times c)}$$

In eq 7, \(dN\) denotes the number of water molecules at \(r\); \(dr\) is the spacing in Å; \(4\pi r^2 \, dr\) is the volume of the spherical shell; \(N\) refers to the overall water molecule count; and \(a \times b \times c\) represents the model volume.

The hydrophobic groups of wetting agents are adsorbed on the surface of bituminous coal, and the hydrophilic groups of wetting agents are adsorbed on the surface of water; water molecule count on the surface of the bituminous coal can be determined by analyzing the water molecule count in the vicinity of the hydrophilic groups. With a greater count of water molecules on the surface of bituminous coal, the wetting effect of bituminous coal is better. The water molecule count around the hydrophilic groups at a distance \(r\) is calculated by formula 8. The \(r\) was set as 20 Å. The number of water molecules near the hydrophilic groups in SDS, SDDS, and SDBS simulation systems are 198, 189, and 175, respectively.

$$dN = \frac{g(r) \times N \times 4\pi r^2 \, dr}{a \times b \times c}$$

By comparing the interaction energy between the wetting agent solution and bituminous coal, diffusion coefficient of the water molecule, and water molecule count on the surface of bituminous coal, the wettablility of three wetting agents for bituminous coal is identified to follow the trend SDS > SDDS > SDBS.

### 4. CONCLUSIONS

The wetting processes of coal dust are adhesion, spreading, and immersion. The greater the wetting work, spreading work, and immersion work, the better the wetting performance of bituminous coal. The wettablility of three wetting agents toward bituminous coal has been established in the following...
trend: SDS > SDDS > SDBS. Compared with previous coal dust-wetting experiments, the preferred experimental method of coal dust wetting agents is improved.

The wetting agent is added to the water, resulting in a decrease in the cohesiveness between the water molecules. Under the action of electrostatic force and hydrogen bond, the water molecules are adsorbed on the hydrophilic group of the wetting agent and the surface of the bituminous coal, which improves the wettability of bituminous coal.

In the MD simulation, the wettability of different wetting agents to bituminous coal is determined based on the intermolecular interaction energy, water molecule diffusion coefficient, and water molecule count in the vicinity of the hydrophilic groups. The wetting trend of three wetting agents to bituminous coal shows the same trend compared to experimental conclusions, which offers a novel insight into preferring wetting agents for coal dust. It avoids the disadvantages of a long experimental cycle, cumbersome process, and time and labor consumption.

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