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Effect of different concentrations of surfactant on the wettability of coal by molecular dynamics simulation

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ABSTRACT

Anionic surfactant sodium dodecyl benzene sulfonate (SDBS) at varying concentrations was selected to investigate the influence on the wettability of Zhaozhuang Coal by molecular dynamics simulation. Six groups of water/surfactant/coal systems with different concentrations were constructed. The influence of surfactant with different concentrations on the wettability of coal was concluded by analyzing various properties from the energetic behaviors to the dynamic characteristics. The results show that the interfacial tension decreases sharply and then rises slowly with the increase of SDBS surfactant concentration, obtaining that surfactants can obviously reduce the interfacial tension. The surfactant molecules could be detected at the water/coal interface through analyzing the system's relative concentration distribution. In addition, the difference in the wettability of surfactants on coal surfaces is caused by the spatial distribution differences of alkyl chains and the benzene ring of the surfactant molecules. And the negative interaction energy between SDBS and the coal surface indicates that adsorption process is spontaneous. Furthermore, it is of great practical significance for improving the dust reduction effect and reducing the disaster of coal dust by exploring the effects of surfactant molecules on the wettability of coal.

1. Introduction

In recent years, although the development of coal mining methods and technologies has promoted the improvement of coal mine mechanization, it also has caused serious environmental issues. Coal dust disaster is still a serious threat in coal mining. The large amount of coal dust is suspended in air or deposited in the roadway, and it not only reduces the visibility of the working face, pollutes the working environment, but also causes pneumoconiosis if workers are continuously exposed to respirable coal dust of high concentrations, which seriously threatens the health of the miners [1]. Moreover, the deposited coal dust may explode and cause other serious casualties under certain conditions [2]. At present, coal seam water injection to suppress dust and sprinkling water for dust elimination or a combination of the two measures have been widely used [3]. However, due to the presence of large numbers of hydrophobic groups such as aliphatic hydrocarbons and aromatic hydrocarbons on the surface of coal dust, the control effect on respiratory coal dust is not over 50% when the sprinkling water technique is used [4]. In general, non-polar group has main effect on hydrophobic and chemical adsorption capacity, therefore, the surface tension of pure water is too large to effectively wet the coal dust [5]. Experiments show that surfactants can reduce the surface tension of water and enhance the ability of aqueous solutions to diffuse on coal surfaces [6]. This is very beneficial to coal seam water infusion, spray sprinkling and other dust control work in coal mine. Wang et al. analyzed the effects of different kinds of wetting agents on the efficiency of dustfall by measuring contact angles of different wetting agents on the surface of coal sample [7]. Crawford et al. investigated the influence of surfactants on the surface characteristics of different coals and found that adding surfactants can reduce the contact angle and improve the wetting effect of coal obviously [8]. By a large number of experiments, Paria and Khilar explored the process that the adsorption of surfactant on the hydrophilic solid liquid interface, and it demonstrated that the dynamics and equilibrium adsorption of different types of surfactants at the solid-liquid interface depend on the properties of the surfactant and solid surface [9]. The wetting effect of various surfactants is different due to the physical and chemical properties of the solid surface. The majority of cationic surfactants are derivatives of organic amines. When the solution is contacted with the

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coal surface, it becomes acidic and organic amines are easily precipitated, so the solutions lose the surface active effect. Therefore, cationic surfactants are inappropriate for coal seam water injection, but anionic surfactants are widely used in related experimental studies. Xu et al. studied the influence of four kinds of anionic surfactants such as SDBS on oil-water interfacial tension, and put forward the mechanism of influence of molecular structure on the interfacial tension [10]. In addition, the effect of SDBS on the properties of oil-water interface at different temperatures was investigated by Wang et al., and it was obtained that SDBS maintains a low interfacial tension in a certain temperature range [11]. Chen et al. discovered that SDBS can greatly improve the wetting properties of coal by investigating the effect of SDBS on coal wettability [12]. Therefore, the surfactant selected in the tests is an anionic surfactant called sodium dodecyl benzene sulfonate (SDBS).

Molecular dynamic simulation is a powerful method, and the method not only has a big application potential in researching the function mechanism between the reagents and minerals, but also enables us to study the dynamic process from molecular perspective [13]. Recently, many scholars have explored the aggregation morphology of surfactant molecules at the interface from the molecular perspective to explain the microcosmic mechanism of surfactants [14–16]. Sun et al. simulated the adsorption and self-assembly of SDBS surfactant on Nano graphene surface based on the molecular dynamics simulation methods, and then explored the interface morphology at different adsorption concentrations [17]. Li et al. studied the adsorption of two common anionic surfactants (such as SDBS) at the oil-water interface by using molecular simulations and found that the hydrophobic chains of surfactants were helpful to reduce the interfacial tension [18]. Zhou et al. studied the effect of adsorption of different types of surfactants on the surface wettability and flow resistance of the slit Nano-pore by molecular dynamics method, meanwhile, the relationship between molecular structure and properties of surfactants was investigated by calculating interfacial formation energy, which supplemented the mechanism of the influence of surfactants on flow resistance [19]. All these researches illustrated that the molecular dynamics simulation has become a valuable tool to investigate the adsorption and wettability phenomenon. However, there are few reports about the adsorption state of surfactants on coal surfaces due to the complex chemical structure of coal [20,21]. The research on the adsorption of surfactant on coal surface and the effects of surfactants on coal wettability by molecular dynamics method can provide dynamical, energetic, and structural information, while the information cannot be obtained by experimental methods. Guo et al. studied the effect of surfactant adsorbing different hydrophilic groups on the wettability of lignite surface according to molecular dynamics simulation, it was found that the adsorption of surfactant on lignite surface was physical adsorption, and the van der Waals interaction plays an important role in the adsorption process [22]. Lv et al. used the molecular dynamics simulation methods to study the adsorption behavior of surfactants on low-rank coals, found that adsorption was mainly affected by polar interactions between surfactants and the hydrophilic sites on the coal surface [23]. Zhang et al. investigated the effects of surfactant on the adsorption behavior and wettability of lignite by molecular dynamics simulation, which detected that surfactants can change the interaction force between water and lignite [24].

In order to improve the efficiency of surfactants and enhance the coal dust suppression by coal seam water injection or spray spraying, it is necessary to explore the influence of surfactants concentration on dust reduction effect or to develop new highly effective surfactants. Nevertheless, understanding the interaction mechanism of surfactant molecules with coal and water molecules is the key to solving these problems. Therefore, the objective of this paper is to better understand the influence of surfactant on wettability of coal, thereby significantly improving the effect of inhibiting coal dust. Meanwhile, the interaction of surfactant molecules with coal and water molecules in the simulation systems at varying concentrations of sodium dodecyl benzene sulfonate surfactant are investigated by molecular dynamics simulation. By quantifying the molecular structural and dynamical behavior of the water-surfactant-coal systems, the micro mechanism of wettability alteration between SDBS and the Zhaozhuang coal are revealed. The obtained results are helpful to screen and develop new surfactants as well as increase the hydrophilicity of the Zhaozhuang coal. Moreover, the molecular level studies based on molecular dynamics simulations provide a more comprehensive understanding for the influence of surfactants on wettability of coal. And it also provides technical ideas to study the new surfactants and has great application value for the prevention of dust poisoning in mines.

2. Experimental and simulated methods

2.1. Coal samples preparation

The coal samples were obtained from the No. 3 coal of Zhaozhuang Mine in Shanxi province, China. The fresh coal samples were vacuum-sealed and immediately sent to laboratory for analysis. The samples were pulverized and screened to pass a sieve size of 60–80 meshes (particle size 200–250 μm), followed by the conventional analyses. The proximate analysis was conducted by using the GF-A2000 auto proximate analyzer and following the Chinese National Standard GB/T 212–2008. The true density of coal samples was measured according to the method described in GB/T 217-2008. And the results of proximate and ultimate analysis of the Zhaozhuang coal sample are presented in Table 1.

2.2. Coal molecular model

The construction of the Zhaozhuang coal molecular model requires the ultimate analysis and 13C NMR analysis of the prepared coal sample. Their atoms ratios and 13C NMR analysis results are shown in Tables 2 and 3. Since the physical and chemical structure of coal matrix is very complex, the Zhaozhuang coal molecular model constructed previously by research group was used in this paper, as shown in Fig. 1 [25]. The structure of Zhaozhuang coal model was optimized. Fig. 2 shows the energy-minimum conformation of structural model of the coal sample from Zhaozhuang.

2.3. Molecular dynamics simulation

Molecular dynamics simulations were conducted by using the Materials Studio 8.0 software package. All the simulations were carried out under the COMPASS force field [26]. The equation of COMPASS force field can be represented as follows:

$$E_{total} = E_{bond} + E_{angle} + E_{oop} + E_{torson} + E_{cross} + E_{electrostatic} + E_{VAW} \quad (1)$$

where E_{bond}, E_{angle}, E_{oop}, $E_{torsion}$ and E_{cross} are the bond stretching energy, angle bending energy, out-of-plane angle coordinates, bond torsion energy and cross-term interacting energy, respectively; and $E_{electrostatic}$ and E_{VDW} the electrostatic interaction and van der Waals interaction, respectively.

2.3.1. Simulation systems

In this paper, a simplified surfactants model was used to simulate in the surfactant/water/coal simulation systems, and the quoted structure model of surfactant is shown in Fig. 3a [27]. By changing the number of surfactants to reflect the behavior of