

Effect of Moisture on Methane Adsorption Characteristics of Long-Flame Coal

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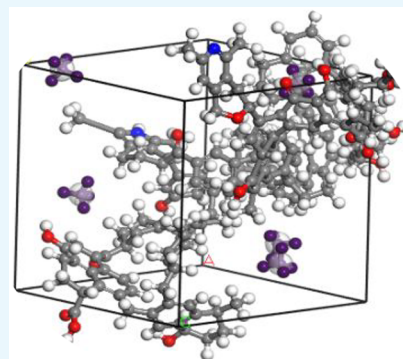
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ABSTRACT: Long-flame coal is a bituminous coal with the lowest metamorphic degree, accounting for 16.1% of China's coal reserves. With increases in mining depths and intensities, mine gas disasters related to the mining of long-flame coal are becoming increasingly serious. Therefore, the exploration of the effect of moisture on the adsorption of methane in coal can provide support for popularizing the application of hydraulic measures in long-flame coal mining areas. In this paper, a molecular structure model of long-flame coal was established by molecular dynamics and the Monte Carlo method. The adsorption characteristics of methane in long-flame coal structures under different pressures were simulated, and the effects of different amounts of water on the methane adsorption and adsorption heat were explored. The results show that, under the same adsorption equilibrium pressure, the methane adsorption rate decreases with increasing water content, and with increasing adsorption equilibrium pressure, the adsorption capacity of methane increases gradually; this increasing trend is in agreement with the Langmuir equation. The water adsorption of coal is greater than the methane adsorption of coal. With the increase in the number of water molecules, when coal-based molecules adsorb methane and then adsorb water molecules, the adsorption heat of methane is reduced, and the desorption of methane molecules is promoted.



1. INTRODUCTION

China is not only the largest producer and consumer of coal in the world but also one of the countries with the most serious coal mine disasters in the world.¹ According to the data of the National Bureau of Statistics, China's coal output shows an increasing trend year-over-year. In the 15 years from 2005 to 2020, China's coal output increased from 2.15 billion tons to 3.9 billion tons. With the increase in coal production, gas accidents are also increasing year-over-year.² Gas control is still the "first difficult problem" in coal mine production. In the past, gas accidents mainly occurred in the mining of medium and high metamorphic coal seams. However, with the increase in mining depth and intensity, gas disasters in low metamorphic coal seams are becoming increasingly serious.³ Long-flame coal is the lowest metamorphic bituminous coal, accounting for 16.1% of China's coal reserves, the largest constituent coal type. Therefore, research on the control of the gas disasters of long-flame coal is particularly important.

To solve the threat of gas disasters to coal production, scholars have carried out a series of studies, which have shown that hydraulic measures are more effective in controlling gas disasters than other measures. Hydraulic measures can be divided into fracturing types and cutting types.⁴ The former mainly produces cracks in boreholes by applying high-pressure water, while the latter increases the amount of coal produced by boreholes through hydraulic cutting and hydraulic punching.⁵ Hydraulic measures can effectively reduce the

internal energy of gas and the bearing stress of coal, so they are widely used. Therefore, it is of great significance to study the effect of moisture on gas adsorption in coal.

At present, the research on the effects of the adsorption and desorption of methane in coal by water mostly focuses on macro-engineering practices. Wang et al. applied hydraulic punching technology to soft and low permeability outburst coal seams and achieved remarkable results.⁶ Wang applied high-pressure hydraulic slotting and fracturing experiments to the Aibeigou mining area in Xinjiang, and the amount of drilling was reduced.⁷ Yang et al. investigated hydraulic cutting styles in boreholes and the optimal equivalent borehole diameter after discharging pulverized coal particles.⁸ Zhu et al. established the adsorption isotherm of methane under different water contents, and the results showed that the presence of water led to a sharp decrease in methane adsorption.⁹ Guo et al. studied the influence of moisture on the adsorption characteristics of low-rank coal and found that moisture obviously inhibited the gas adsorption capacity of

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low-rank coal and that the inhibition degree increased with increasing moisture content.¹⁰ Although scholars have performed much research on the effect of moisture on gas adsorption in coal, most of them focus on high metamorphic coal with serious disasters, but there are few studies on low metamorphic coal, especially long-flame coal.

On the basis of previous studies, this paper studies the interaction between methane and moisture in long-flame coal, aiming to determine the adsorption characteristics of methane in the structure of long-flame coal under different pressures and reveal the effects of different moisture contents on methane adsorption and adsorption heat change. The research conclusions provide support for the application of hydraulic measures in the treatment of low metamorphic coal and gas disasters.

2. RESEARCH METHOD

2.1. Molecular Simulation Method. Molecular simulation methods mainly include molecular mechanics, molecular dynamics, and Monte Carlo methods.¹¹ Classical Newtonian mechanics is at the core of molecular mechanics, and the molecular force field contains a large number of parameters that can be calculated by quantum mechanics. After the force field is selected, the potential energy of various possible conformations of molecules can be obtained from the force field parameters, among which the conformation with the lowest potential energy is the stable conformation, and the complex molecular stable conformation can be calculated by molecular mechanics method.¹² The basic principle of molecular dynamics simulation is to calculate the potential energy of a system as a particle system composed of molecules and atoms. In molecular dynamics simulations, periodic boundary conditions are necessary, and the periodic boundary conditions are a periodic mirror system, which maintains a constant number of particles.¹³ The Monte Carlo method is a computational simulation method applied to dense systems. Using random sampling to address the problem, the statistical approximate solution is obtained through the experimental calculation of the model. The basic idea behind the Monte Carlo method is the Metropolis sampling method.¹⁴ The Metropolis sampling method overcomes the shortcomings of simple sampling methods to achieve the purpose of selective sampling.¹⁵ In this paper, molecular dynamics and Monte Carlo methods are used to explore the effect of moisture on the methane adsorption of coal.

2.2. Model Building. In this paper, a macromolecular structure is drawn by ChemDraw software and imported into the Materials studio software. The Forcite module and Sorption module in the software are used for optimization and molecular adsorption. The Forcite module mainly optimizes and calculates the energy of a periodic system and obtains the result file of energy optimization; it is a classical molecular mechanics tool that includes force field, charge distribution, and other parameter settings.¹⁶ The Sorption module uses the Monte Carlo method to simulate the adsorption characteristics and adsorption isotherms of substances, and the model is modified on the basis of the molecular structure model of long-flame coal constructed by Lian.¹⁷ The selected molecular substrate of long-flame coal is an amorphous molecular structure of an aromatic skeleton composed of 407 atoms, which mainly includes four elements: carbon, hydrogen, nitrogen, and oxygen. The structural

molecular formula is $C_{189}H_{196}N_2O_2$. The coal-based molecular structure is shown in Figure 1.

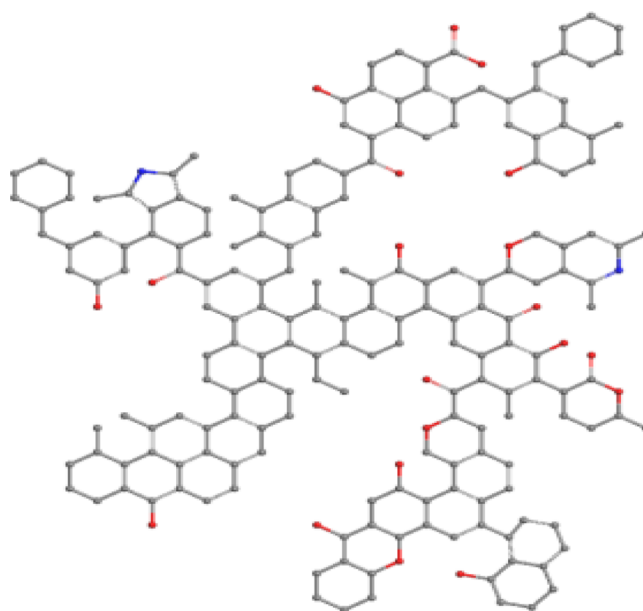


Figure 1. Molecular structure of long-flame coal.

The molecular structure is hydrogenated and saturated, and the Clean module is optimized until the structure is initially stable; the structure is obtained as shown in Figure 2. The

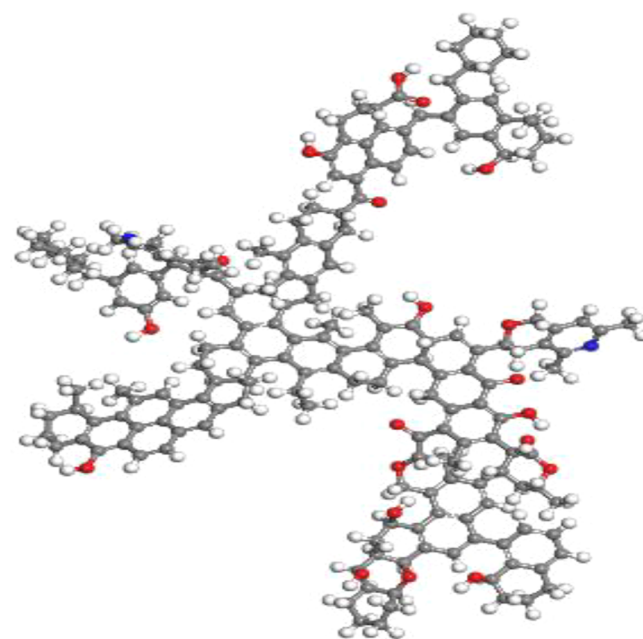


Figure 2. Coal-based molecular structure optimized by Clean.

Forcite module is used to optimize the molecular dynamics, and the optimization parameters are set as follows: the task is set to Geometry Optimization, the precision is set to Fine, the selected force field is COMPASS, and the interaction force is calculated by the Ewald summation method (because the Geometry task can only get the local energy minimum configuration). In order to obtain the lowest energy configuration on the whole potential energy surface, the

molecular model needs to be globally optimized by annealing dynamics simulation. The globally optimized molecular model is shown in Figure 3, when the adsorption configuration energy

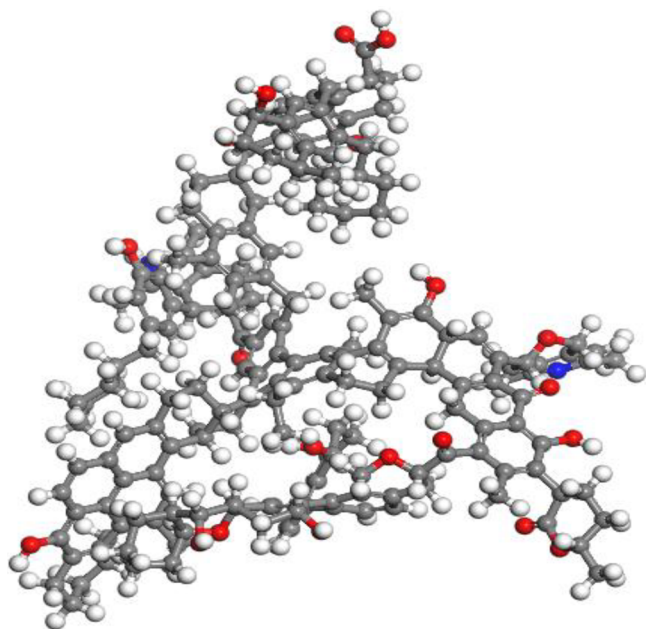


Figure 3. Molecular structure after annealing.

of long-flame coal is the lowest. The periodic boundary conditions are established for the optimized molecular structure, and the density is optimized. The optimized density is 1.24 g/cm³, which is within the desired experimental range.^{18,19} The optimized structure is shown in Figure 4.

The optimized model is a periodic boundary model (Figure 5). The size parameters of x , y , and z are $1.56 \times 1.56 \times 1.56$ nm³, and $\alpha = \beta = \gamma = 90^\circ$. The molecular structure is optimized by first principle, and the energy changes before and after long-flame coal structure optimization are compared as shown in Table 1.

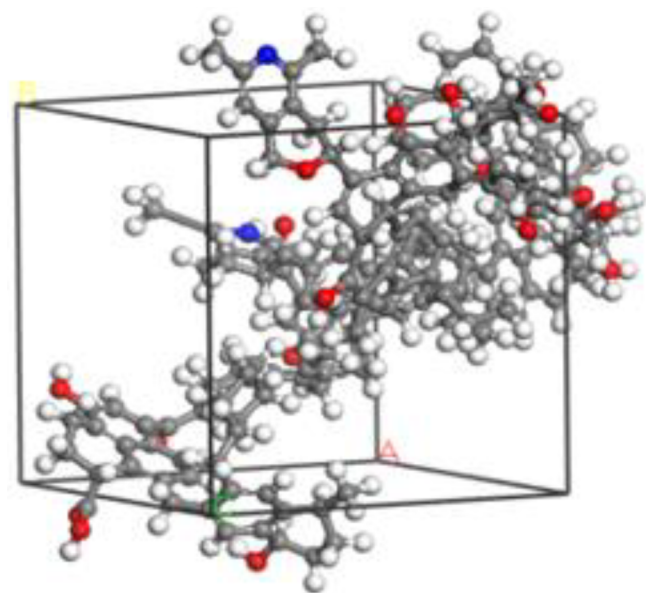


Figure 4. Molecular structure optimized by Forcite.

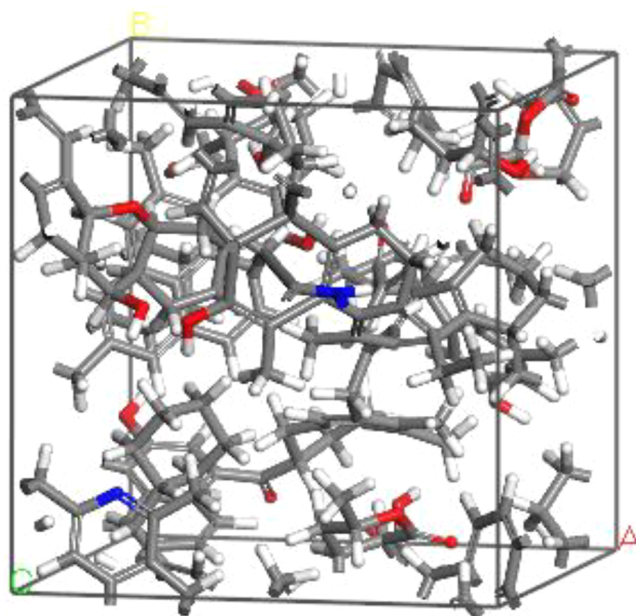


Figure 5. Final adsorption configuration of long-flame coal (color in the figures: O, red; H, white; N, dark blue).

Table 1. Energy Comparison of Long-Flame Coal before and after Molecular Structure Optimization

| | energy (kcal/mol) | |
|-------------------------|-------------------|-----------------|
| | initial structure | final structure |
| total energy | 1411.81 | 846.07 |
| valence energy | 945.96 | 626.78 |
| bond energy | 318.96 | 220.18 |
| angular energy | 393.33 | 133.82 |
| torsion energy | 227.60 | 174.21 |
| inversion energy | 6.1 | 1.90 |
| nonbonding energy | 465.85 | 96.67 |
| hydrogen bonding energy | 0 | 0 |
| van der Waals force | 465.86 | 96.67 |
| Coulomb energy | 0 | 0 |

The total energy of the force field comprises three types of energy: bonding interaction energy, nonbonding interaction energy, and cross energy.²⁰ The total energy composition is as follows:

$$E_{\text{Total}} = E_{\text{valence}} + E_{\text{nonbond}} \quad (1)$$

Among them, the bonding interaction energy comprises bond energy, angular energy, torsion energy, and inversion energy; the energy composition is as follows:

$$E_{\text{valence}} = E_{\text{bond}} + E_{\text{angular}} + E_{\text{torsion}} + E_{\text{inversion}} \quad (2)$$

while the nonbonding energy comprises van der Waals energy and hydrogen bonding energy.²¹ In the nonbonding energy, the main force is the van der Waals force. The nonbonding energy composition is as follows:

$$E_{\text{nonbond}} = E_{\text{vvd}} + E_{\text{Coulomb}} + E_{\text{H bond}} \quad (3)$$

Table 1 shows that, after molecular mechanics optimization and molecular dynamics optimization, the total energy and each energy of the long-flame coal structure obviously decrease. The initial total energy of the structure is 1411.81 kcal/mol, and the final total energy of the structure is reduced

to 846.07 kcal/mol after gradual optimization. In the nonbond energy, the main force is van der Waals energy; hydrogen bond energy and Coulomb energy are 0. The van der Waals force in the coal-based molecular system obviously decreases. This shows that van der Waals forces play a significant role in the stability of the coal molecular structure.

3. RESULTS AND DISCUSSION

3.1. Effect of Pressure on CH₄ Adsorption of Long-Flame Coal. Under the conditions of 30 °C and an adsorption equilibrium pressure of 1 MPa, the methane adsorption of the optimized molecular model was simulated using the Locate task item in the Sorption module. The Metropolis sampling method was used; the precision was set to Fine, the force field was set to Dreiding. The charge was set to Use current. The interaction force and van der Waals forces were summed by Ewald and Atom methods. The molecular structure of long-flame coal reached a saturated state after adsorbing five CH₄ molecules. Figure 6 shows the adsorption of five CH₄ molecules by long-flame coal molecules.

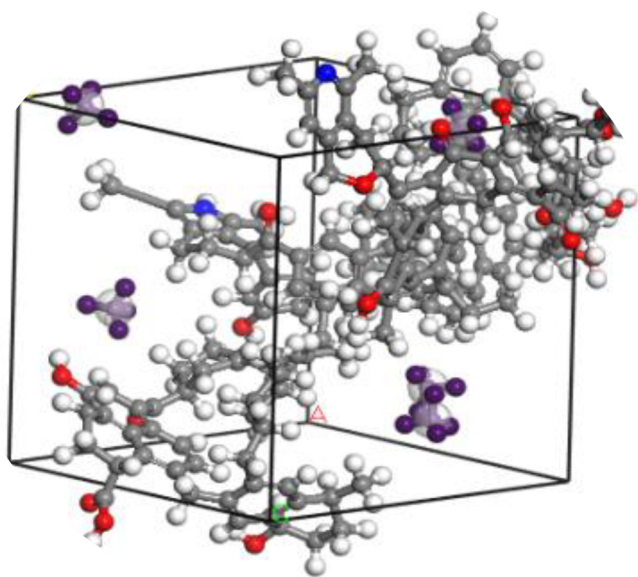


Figure 6. Long-flame coal molecules adsorbing 5 CH₄ molecules.

In molecular simulations, the adsorption equilibrium pressure is generally expressed by fugacity.^{22,23} Fugacity represents the effective pressure of real gas and is a concept produced by considering an ideal gas with the same chemical potential under the same conditions.²⁴ The fugacity coefficient is an important parameter for measuring the deviation between a real gas and an ideal gas. Fugacity and pressure are similar in real gas at low pressure, but there is a great difference between them under high pressure, so it is necessary to convert pressure into fugacity, which is calculated by the Peng–Robinson equation of state. After the conversion of pressure into fugacity, the curve of fugacity changing with increasing pressure is shown in Figure 7.

According to Figure 7, the two curves almost coincide at a temperature of 30 °C, and the gap between the two curves gradually widens after 2.5 MPa. When the pressure is lower than 2.5 MPa, there is little difference between methane fugacity and water fugacity. With increasing pressure, the difference between the methane fugacity and water fugacity

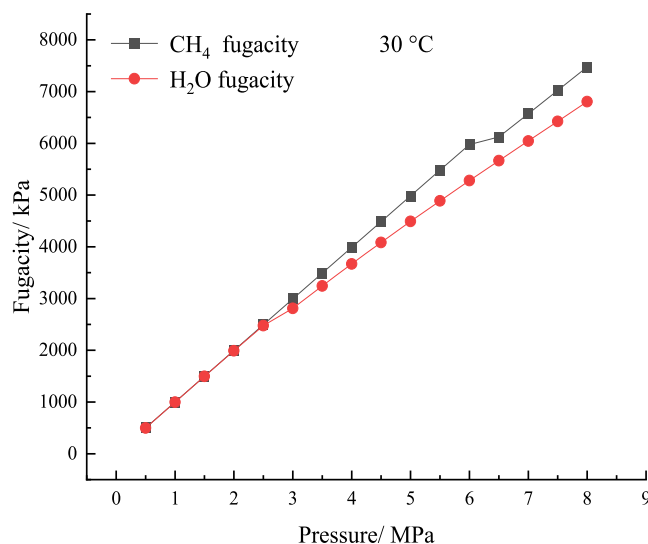


Figure 7. Variation trend of fugacity with pressure.

and the corresponding pressure increases, and the difference between the fugacity and pressure increases gradually in the range of 2.5–8 MPa. This result reflects that there is no significant difference in the fugacity in the low-pressure region, but there is a great difference in the high-pressure range. Therefore, when the equilibrium pressure of methane adsorption is lower than 2.5 MPa, fugacity and pressure do not need to be converted, but when methane adsorption is above 2.5 MPa, the conversion between pressure and fugacity is needed.

Because the simulated molecular weight is that of the molecule under absolute adsorption, it includes not only the amount of gas adsorbed in the micropores but also the amount of gas dissociated in the micropores.²⁵ The excess adsorption capacity represents the gas amount of the adsorption phase on the surface of coal and rock micropores, excluding the bulk adsorption capacity, which represents the amount of gas dissociated in the micropores. Because the isothermal adsorption capacity of methane measured in the laboratory is the excess adsorption capacity, the absolute adsorption capacity should be converted into the excess adsorption capacity.²⁶

$$\rho_{\text{excess}} = \rho_{\text{absolute}} - \rho_{\text{bulk}} \quad (4)$$

where ρ_{excess} is excess adsorption (mmol/g); ρ_{absolute} is absolute adsorption (mmol/g); ρ_{bulk} is bulk adsorption (mmol/g).

The adsorption capacity of methane is simulated in the process of adsorption saturation, and the adsorption capacity of methane under different adsorption equilibrium pressures is shown in Figure 8.

Figure 8 shows that the excess adsorption capacity of methane increases with increasing adsorption equilibrium pressure at 30 °C. According to the adsorption curve, the adsorption capacity of methane increases rapidly from 0.58 to 0.8 mmol/g in the range of 0–2 MPa and slows down in the range of 2–4 MPa. In the range of 4–8 MPa, the excess adsorption capacity of methane gradually tends toward equilibrium. This is because, with increasing pressure, the extension of the molecular structure increases, and the free paths between methane molecules decrease such that the number of adsorption sites for methane increases.²⁷ Thus, the probability of being adsorbed is greater, resulting in an increase

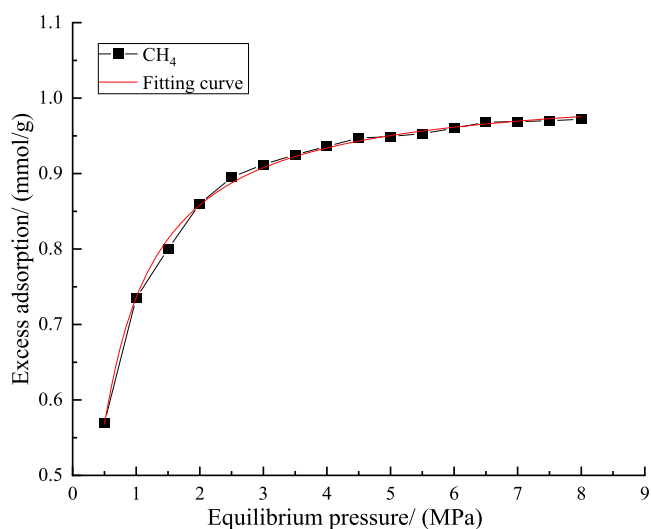


Figure 8. Excess adsorption capacity of CH₄ under different adsorption equilibrium pressures.

in the adsorption capacities of methane molecules. When the pressure is large enough, the adsorption capacities gradually tend to be saturated, and the processes of adsorption and desorption reach dynamic equilibrium.

3.2. Effect of Moisture on CH₄ Adsorption of Long-Flame Coal. The external conditions affecting gas adsorption mainly include temperature, pressure, moisture, and so on.²⁸ Water molecules are polar molecules, which makes it easier for them to occupy methane adsorption sites and adsorb onto the surfaces of coal pores, resulting in a decrease in methane adsorption.²⁹ Using the Sorption module of Materials Studio, the molecular model first adsorbs methane molecules and then adsorbs water molecules under the function of the Locate task. Under the condition of 30 °C, the changes in the adsorption energy and adsorption heat of the water molecules adsorbed by the coal-based molecular structures of adsorbed methane molecules and unadsorbed methane molecules are studied under different pressures. The range of pressure settings is 0.5–8 MPa.

It can be seen from Figure 9 that the energy of long-flame coal is the lowest when adsorbing five methane molecules, which corresponds to the lowest energy configuration, indicating that the coal structure is saturated after adsorbing five methane molecules. With the increase in the number of adsorbed molecules, the total energy decreases gradually, and the trend of van der Waals energy, which plays an important role in the total energy, is basically the same as that of the total energy. When the long-flame coal molecule adsorbs the fourth methane molecule, the system energy is the lowest and reaches the optimal state. It is worth noting the following: whatever long-flame coal molecular structure on the adsorption of methane or moisture, the overall potential energy presents a downward trend; this is because the potential energy has relativity. When one assumes that the adsorption potential energy is zero, a position larger than the location of the potential energy is positive, and the potential energy smaller than this position is negative.

Figure 10 shows the energy curve of long-flame coal molecules adsorbing water molecules. When long-flame coal molecules adsorb the ninth water molecule, the system energy is the lowest and reaches the optimal state. Different from adsorbing methane molecules, not only van der Waals energy

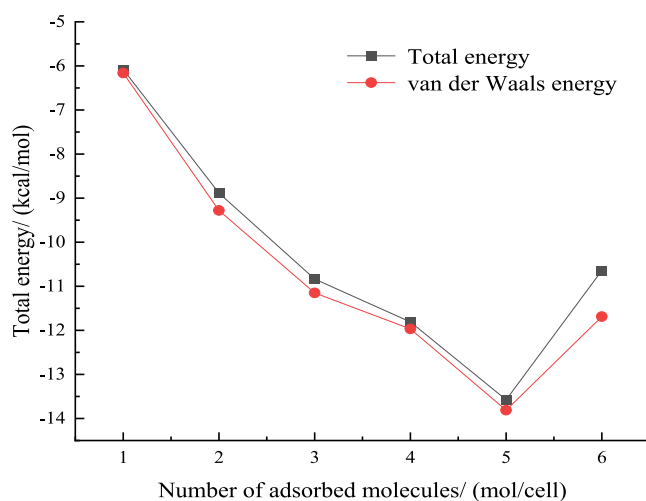


Figure 9. Energy curve of coal-based molecules adsorbing methane molecules.

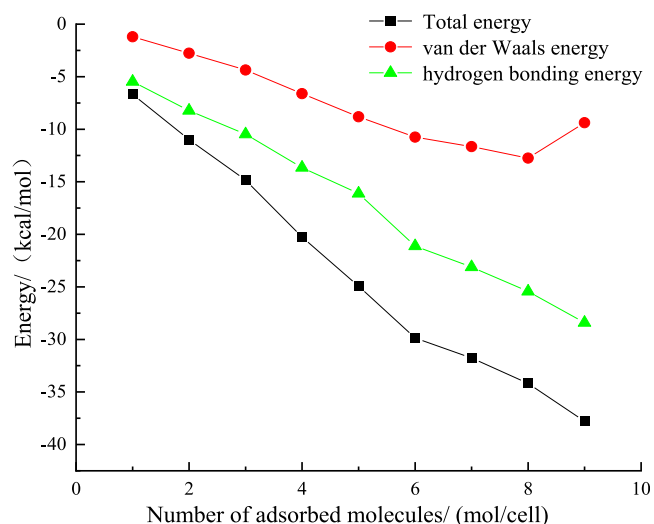


Figure 10. Energy curve of coal-based molecules after adsorption of water molecules.

but also hydrogen bonding energy play a major role in adsorbing water molecules. In the process of structural optimization, the van der Waals energy and hydrogen bonding energy obviously decrease, and the total energy decreases. With the increase of adsorbed water molecules, hydrogen bond energy plays a more and more important role, while van der Waals energy plays a more and more weak role. Although van der Waals energy increases slightly in the later stage, the overall energy still shows a gradual decline due to a large decrease in hydrogen bond energy.

Figure 11 shows the energy change of the molecular structure of long-flame coal after adsorbing water molecules on the basis of adsorbing different methane molecules. With the increase in adsorbed water molecules, the total energy of the molecular structure of long-flame coal decreases. According to the adsorption heat curve of Figure 12, when long-flame coal molecules adsorb methane molecules, the adsorption heat remains within the range of 5.4–5.5 kcal/mol with increasing adsorption equilibrium pressure, indicating that there is no direct relationship between the adsorption equilibrium pressure and methane adsorption heat. Figure 13 shows the

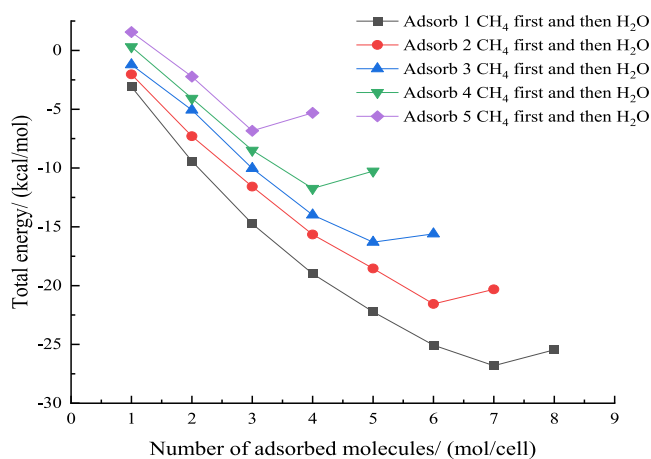


Figure 11. Energy change of the molecular structure of long-flame coal after moisture adsorption based on methane adsorption.

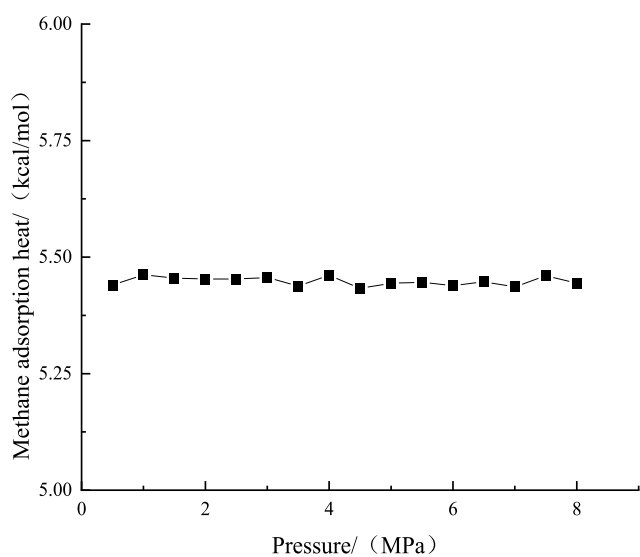


Figure 12. Adsorption heat of CH_4 under different adsorption equilibrium pressures.

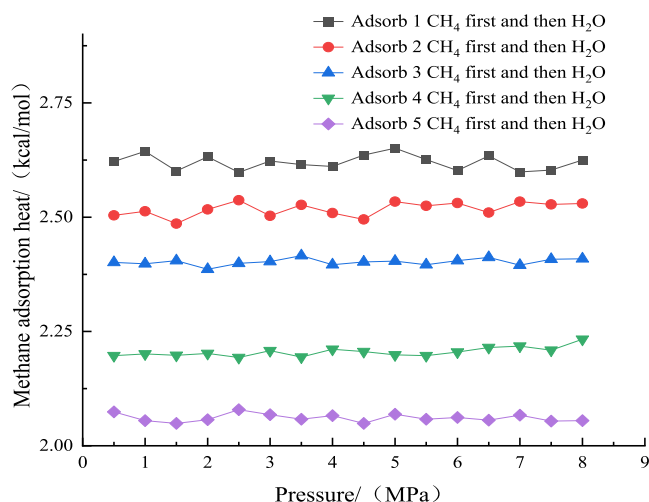


Figure 13. Adsorption heat change of moisture adsorption by coal-based molecules after methane adsorption.

change in the adsorption heat of long-flame coal molecules on the basis of adsorption of methane molecules and then the

adsorption of water molecules, a process that results in the adsorption heat of methane decreasing to 2–3 kcal/mol, which indicates that long-flame coal molecules first adsorb methane and then adsorb water under different adsorption equilibrium pressures. With the increase in the number of adsorbed water molecules, the methane adsorption heat and the methane adsorption capacity decrease.

At 30 °C, the change in methane adsorption with different moisture contents is shown in Figure 14.

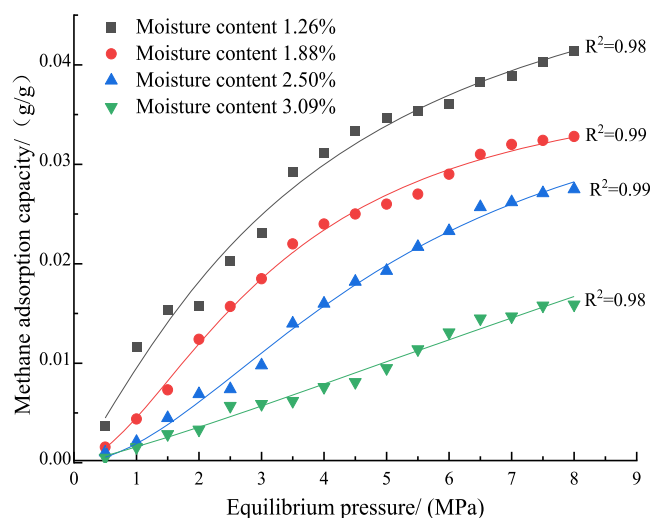


Figure 14. Methane adsorption under different moisture contents.

The adsorption curve is consistent with the Langmuir curve. When the adsorption equilibrium pressure is 0–3 MPa, the methane adsorption rate of long-flame coal increases rapidly, and with increasing adsorption equilibrium pressure, the methane adsorption rate decreases and gradually tends to smooth. With increasing moisture content, the methane adsorption capacity decreases, and when the moisture content is 1.2%, the limit of the adsorption capacity of methane is 0.04 mol/cell. When the moisture content is 3.08%, the limit of the adsorption capacity decreases to 0.015 mol/cell. With the increase of moisture content, water preferentially selects the oxygen-containing functional groups on the coal surface for adsorption, and then, the adsorbed water molecules can form multilayer adsorption and agglomeration through hydrogen bonding, which occupies the adsorption site of methane on the coal surface. The adsorption capacity of the coal structure to water molecules is better than that of methane; the methane adsorption sites on the surface of the long-flame coal structure decrease, and the methane adsorption capacity decreases. The adsorption capacity of the moisture content of the coal samples is obviously less than that of dry coal samples. The increase in moisture can promote the desorption of adsorbed methane to a certain extent.

3.3. Effect of Moisture on Methane Adsorption Heat.

Adsorption heat is a kind of thermal effect produced in the process of adsorption, and it is an important index for the characterization of the adsorption capacity of methane. The adsorption heat is related to the adsorption strength of a structure surface, and the higher the adsorption heat, the stronger is the adsorption capacity of the structure. Figure 15 shows the adsorption heat curve of methane when the temperature is 30 °C and the adsorption equilibrium pressure is 1.5 MPa.

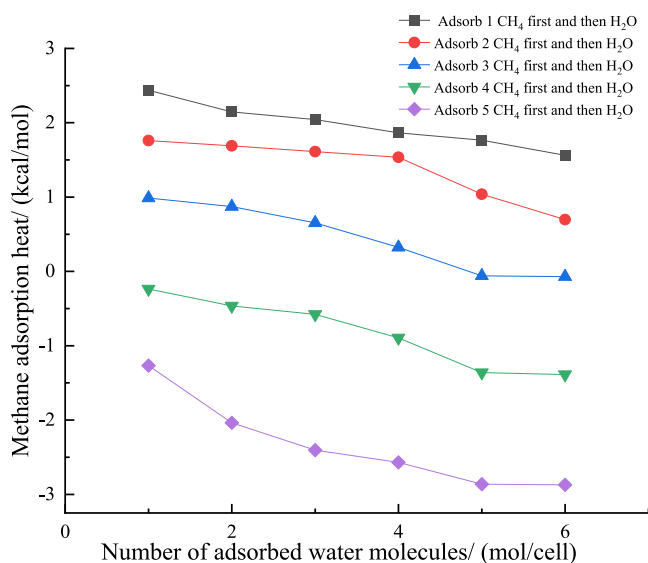


Figure 15. Adsorption heat of methane under the conditions of adsorbing different water molecules.

Figure 15 shows that the adsorption heat of methane decreases gradually with the increase in the number of adsorbed water molecules, and the adsorption heat of methane is in the range of -3 – 2.5 kcal/mol. After the adsorption of the fourth and fifth methane molecule and with the increase in the number of adsorption water molecules, the adsorption heat of methane is negative. Under different adsorption equilibrium pressures, the range of methane adsorption heat is 2 – 3 kcal/mol and that under isobaric pressure is -3 – 3 kcal/mol. When the molecular structure adsorbed more water molecules, the methane adsorption heat was lower and the adsorption capacity of coal for methane was weaker.

4. CONCLUSION

- (1) When the adsorption equilibrium pressure is lower than 2.5 MPa, there is little difference between methane fugacity and water fugacity, but when the adsorption equilibrium pressure exceeds 2.5 MPa, the difference between methane fugacity and water fugacity increases; thus, it is necessary to convert between adsorption equilibrium pressure and water fugacity when simulating methane adsorption and desorption.
- (2) In the dry state, the fixed temperature is 30 °C, and the methane adsorption capacity of long-flame coal increases with increasing adsorption equilibrium pressure, which satisfies the Langmuir adsorption model. The free methane molecules collide with the coal structure surface, and the average free path of free methane decreases. The internal energy increases, and the probability that the methane molecules are captured by the long-flame coal structure surface molecules increases; thus, the methane adsorption capacity of long-flame coal increases.
- (3) van der Waals energy mainly plays a role in the interaction between long-flame coal molecules and methane molecules, which also involves hydrogen bonding energy. After the molecular structure of long-flame coal adsorbs water molecules, the interaction between coal molecules and methane molecules weakens. Thus, an increase in moisture can promote

the desorption of methane in coal to some extent, which lays a theoretical foundation for coalbed methane exploitation.

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Notes

The authors declare no competing financial interest.

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