

Differential Analysis of Various Moisture Phases on N₂ Displacement of CH₄ in Coal

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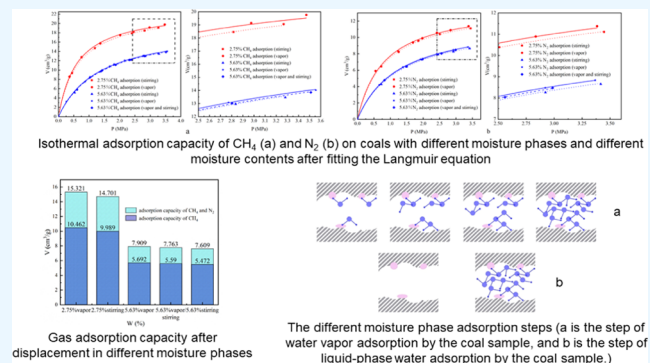
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ABSTRACT: The aim of the study was to elucidate the impact of different moisture phases during gas injection on coalbed methane displacement. The coal samples were treated with two methods: water vapor adsorption and liquid water stirring. The differences in the coal samples treated with various moisture phases during gas injection for coalbed methane displacement were investigated by using the isothermal adsorption curves of CH₄, N₂, and H₂O in coal and N₂ displacement of CH₄ in coal. The results indicate that variations in the gas adsorption capacity of coal are treated with different moisture phases. The gas adsorption capacities and displacement capacities of the coal samples treated with the water vapor adsorption methods are better than those treated with the stirring methods. In the isothermal adsorption experiment, for the coal samples treated with different moisture phases, at a moisture content of 2.75%, the saturated adsorption capacities of CH₄/N₂ are 0.204/0.189 (cm³/g), and at a moisture content of 5.63%, the saturated adsorption capacities of CH₄/N₂ are 0.151/0.139 (cm³/g). In addition, in the displacement experiment, for the coal samples treated with different moisture phases, at a moisture content of 2.75%, the difference in the total gas adsorption capacities is 0.62 cm³/g and the difference in the CH₄ adsorption capacities is 0.473 cm³/g, and at a moisture content of 5.63%, the difference in the total gas adsorption capacities is 0.3 cm³/g and the difference in CH₄ adsorption capacities is 0.22 cm³/g. For the coal samples treated with various moisture phases, the differences in the CH₄/N₂ adsorption and displacement capacities are greater at a moisture content of 2.75% than at 5.63%. Notably, the moisture phase has only a marginal influence on the CH₄ desorption capacity and desorption rate. The study is important to understand the interactions between coal and moisture.



1. INTRODUCTION

Coal seams in China exhibit a complex structure, most of which is soft and has low permeability. To enhance the gas extraction rate from low-permeability coal seams, various methods have been employed to improve permeability,¹ such as hydraulic permeability improvement measures,^{2,3} blasting technology,^{4,5} and gas fracturing technology.⁶ However, there are still some safety concerns and engineering geology limitations. In the late 20th century, CO₂ injection was employed in the San Juan Basin of the United States to enhance the recovery rate of coalbed methane (CO₂-ECBM). As a result of this measure, coalbed methane production increased by 1.5 times and the recovery rate reached 95%,⁷ providing a new direction for gas injection to promote the drainage of coalbed methane.

Scholars at home and abroad have conducted intensive experimental and theoretical research on gas injection to promote coal seam gas drainage. Since the 20th century, Busch,^{8,9} Clarkson,¹⁰ Xiao,¹¹ and Jessen¹² carried out displacement experiments on CO₂, N₂, and mixed gases and compared their effects on methane. Li¹³ suggested that oxygen-containing functional groups on the coal pore surface enhance the

displacement of CH₄ by CO₂. Hu¹⁴ evaluated the effects of different functional groups in coal on its adsorption characteristics.

Nevertheless, the majority of these studies concentrated on dry coal, but the original coal seam contains moisture, which has a great impact on gas adsorption in the coal samples. Therefore, the effect of moisture on the gas adsorption and displacement in coal has been investigated by many scholars. Kang¹⁵ and Zhou¹⁶ found that H₂O inhibited the adsorption capacity of methane on anthracite coal. Han¹⁷ found that water molecules preferentially adsorbed on oxygen functional groups interfere with the adsorption and diffusion of CO₂ and CH₄. Song¹⁸ concluded that water had no significant effect on the pore shape of coal,

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reducing its specific surface area and adsorption capacity. Chen¹⁹ concluded that moisture leads to a decrease in both specific surface area and pore volume, and that the micropores are most affected by the adsorption of moisture in coal.

In order to treat the coal samples with moisture content, scholars from both domestic and international spheres frequently employ the practice of introducing moisture to regulate the moisture content of dry coal samples. Liu²⁰ utilized six saturated salt solutions with different relative humidity levels to regulate the moisture content of the dry coal samples. Jia²¹ and Li²² utilized a vapor generator at different relative pressures to control moisture content. Guo²³ researched a water injection and adsorption device. The moisture sources can be categorized into liquid-phase water and gas-phase water. In this study, with consistent moisture content, the differences in the coal samples treated with vapor (gas-phase water) and stirring (liquid-phase water) during isothermal adsorption of CH₄, N₂, and H₂O in coal and N₂ injection displacement of CH₄ in coal are analyzed.

This manuscript mainly studies the influence of different moisture phases on the isothermal adsorption of N₂/CH₄ on the coal samples and the differences in the effects of N₂ injection to displace CH₄ in the coal samples after the introduction of different phases of moisture to the dry coal samples. First, the coal samples treated with different moisture phases were prepared using different water introduction methods. Then, the differences in the isothermal adsorption of N₂ and CH₄ in the coal samples treated with different moisture phases were investigated. In addition, the different adsorption courses of the two different moisture phases in the interior of the coal matrix were analyzed. Subsequently, the differences in the N₂ displacement of CH₄ in the coal samples treated with various moisture phases were further investigated. Finally, the differences in the influence of various moisture phases on the desorption rate of coalbed methane were summarized. Compared with previous studies, this study provides new insights into the isothermal adsorption and displacement of the coal samples with different moisture contents and the adsorption process of the coal samples with different moisture phases. This study is important to understand the interactions between coal and moisture.

2. EXPERIMENTAL METHODS

2.1. Experimental Sample Collection and Analysis. The coal samples used in this study were extracted from the No. 2 coal seam of the No. 1 working face of the Jiu Lishan coal mine in China. Recently, the exposed gangue-free lump coal from the working face was sealed and brought to the laboratory. The granular pulverized coal of 60–80 mesh (0.18–0.25 mm) was sieved with a standard sieve. Then, the samples were vacuum-degassed and dried at a temperature of 105 °C in an oven for more than 10 h.^{24–26} After these treatments, the coal samples were considered completely moisture-free and could be utilized as blank control. Subsequently, all dried coal samples were removed from the oven and cooled to room temperature before setting aside. The data from the industrial analysis of the coal samples are shown in Table 1.

2.2. Experimental Conditions. To create water-containing coal treated with the water vapor adsorption method (gas-phase water), two saturated salt solutions were used: Mg(NO₃)₂·6H₂O (53% RH) and K₂SO₄ (97% RH).²⁷ The coal samples were equilibrated in saturated salt solutions until the masses of the coal sample remained constant, and the moisture content of the coal samples was calculated. The moisture content was

Table 1. Results of Industrial Analysis of Coal Samples

inherent moisture (%)	ash content (%)	volatility (%)	apparent relative density (g/cm ³)	true relative density (g/cm ³)	porosity (%)
1.01	13.32	7.95	1.52	1.61	5.59

calculated using eq 1. The moisture contents of the coal samples calculated by the water vapor adsorption method were 2.75 and 5.63%

$$W = \frac{m_{\text{moist}} - m_{\text{dry}}}{m_{\text{dry}}} \times 100\% \quad (1)$$

where m_{moist} is the mass of the moist coal (g) and m_{dry} is the mass of the dry coal (g).

In order to achieve moisture contents of 2.75 and 5.63% in the coal samples treated by the stirring method (liquid-phase water), a certain mass of water was dripped into the coal samples while stirring. When the coal samples became loose and homogeneous, stirring was continued for 30 min, and then the samples were wrapped in plastic wrap and allowed to stand at 25 °C. When the mass of the coal samples remained constant, the moisture contents were calculated using eq 1. If the objective moisture content was not reached, then the drip was repeated until it was reached.

The two different moisture content experimental coal samples were treated using two different methods, and five moisture content coals were obtained. Specifically, the five samples included the coal samples with moisture contents of 2.75 and 5.63% treated with water vapor adsorption, the coal samples with moisture contents of 2.75 and 5.63% treated with stirring, and a coal sample with a moisture content of 5.63% treated by combining both stirring and water vapor adsorption methods.

An investigation was conducted to analyze the reasons for the influence of different moisture phases on N₂ displacement coalbed methane experiments through the implementation of single-gas adsorption experiments and gas injection displacement experiments for water-bearing coal treated with different moisture phases.

2.3. Experimental Device. The multicomponent gas displacement system for coal-containing gas consists of six subsystems: high-pressure gas supply system, temperature-controlled adsorption and desorption system, self-storage pressure sensor system, gas component analysis system, vacuum degassing system, and data acquisition system. The experimental device is shown in Figure 1.

2.4. Experimental Steps.

- The experimental conditions were established. The experiments were conducted at 25 °C. The preadsorption equilibrium pressure of CH₄ before displacement was 0.74 MPa. The N₂ injection capacity was kept consistent during the gas injection displacement experiments.
- The airtightness of the experimental equipment was tested. The coal samples were vacuum-degassed and dried. Then, the coal samples were treated with two moisture phases and two moisture contents.
- Isothermal adsorption experiments were conducted on the experimental coal samples. The isothermal adsorption curves of these two gases were fitted using the Langmuir equation (eq 2), yielding the fitting curves for CH₄ and N₂ isothermal adsorption in coal.²⁸ The values of “*a*” and “*b*” for both gases were calculated as follows:

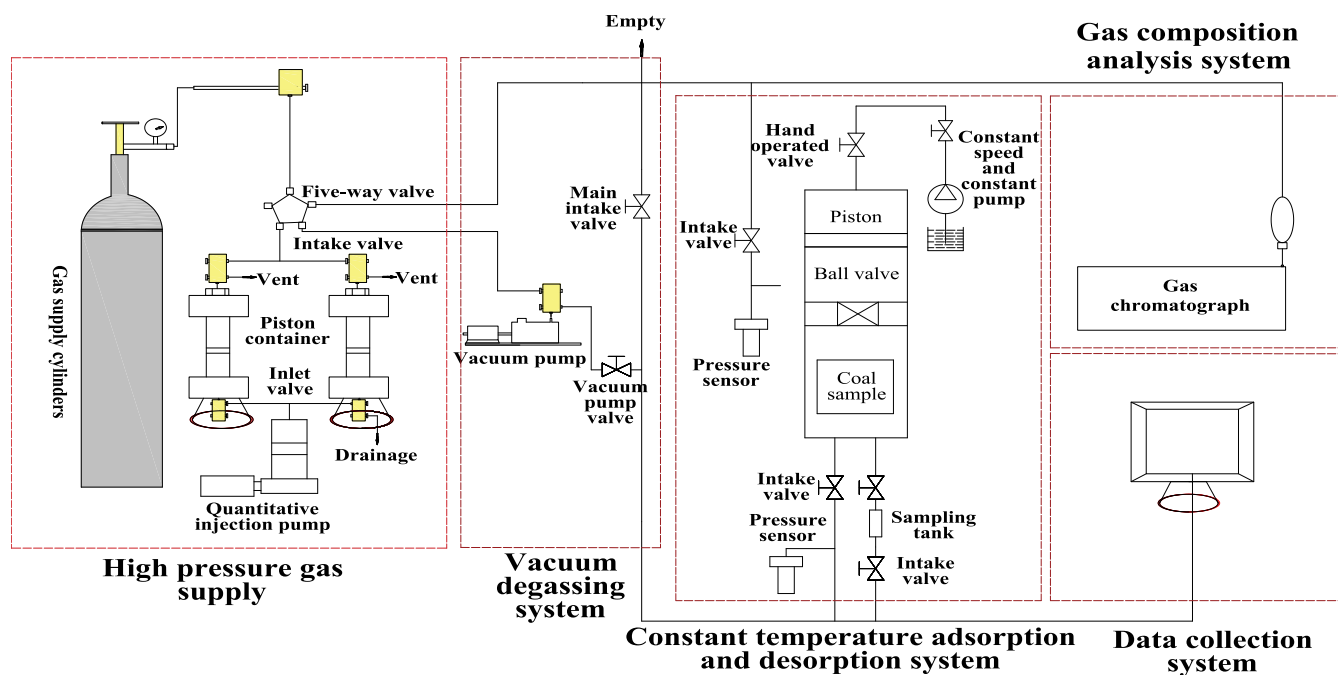


Figure 1. Schematic diagram of the multicomponent gas displacement system.

$$V = \frac{abP}{1 + bP} \quad (2)$$

where P is the gas pressure at adsorption equilibrium, MPa, and V is the volume of gas adsorbed on the surface of the unit mass of the coal sample at a temperature of 25 °C and gas pressure of P . From the experimental data, the values of “ a ” and “ b ” were calculated by fitting the Langmuir equation.

- d. CH₄ from the piston container was injected into the coal sample chamber until the adsorption equilibrium pressure reached a target pressure of 0.74 MPa (preadsorption equilibrium pressure). The coal sample chamber was then pressurized with N₂ to reach the desired pressure level, and the system was allowed to reach the displacement equilibrium. After the displacement equilibrium, the gases in the coal sample chamber were transferred to a gas chromatograph to determine the percent composition of the two gases.
- e. Following the described experimental procedures, single-gas adsorption experiments and gas injection displacement experiments were performed on the five water-containing coal samples under the experiment conditions, as specified.

3. FORMULA CALCULATION

The gas adsorption capacity is determined by calculating the initial gas capacity injected into the coal sample chamber and the difference between the remaining free gas capacity within the coal sample chamber after reaching the adsorption equilibrium. The formulas involved are as follows²⁹

$$V_{zx} = \left(\frac{P_1}{Z_1} - \frac{P_2}{Z_2} \right) \times \frac{273.15 \times (V_r + V_p)}{(273.15 + t_0) \times 0.101325} \quad (3)$$

$$V_y = \frac{273.15 \times V_s \times P}{Z \times (273.15 + t_0) \times 0.101325} \quad (4)$$

$$V_x = V_{zx} - V_y \quad (5)$$

$$Q_x = (V_{zx} - V_y) / m_{\text{dry}} \quad (6)$$

where P_1 and P_2 are the absolute pressures of the gas piston container before and after gas injection, MPa, respectively. Z_1 and Z_2 are the compressibility factors of the gas at pressures P_1 and P_2 , respectively. V_r is the volume of the gas piston container chamber, cm³. V_p is the volume of the utility line, cm³. t_0 is the laboratory temperature, °C. V_s is the remaining volume in the coal sample chamber except for the coal sample, cm³. P is the absolute pressure inside the coal sample chamber at adsorption equilibrium, MPa. Z is the compression factor of the free gas in the coal sample chamber at pressure P . V_x is the adsorbed volume of the gas after adsorption equilibrium at a standard temperature and pressure (STP), cm³. Q_x is the gas adsorption capacity of the gas component at the STP, cm³/g.

With anthracite as the research object, isothermal adsorption experiments of water vapor at 25 °C were carried out, and the Brunauer–Emmett–Teller (BET) model was used to fit the adsorption of H₂O on the coal samples. The initial BET model is unable to accurately characterize the H₂O adsorption equilibrium on coal because it neglects the heterogeneity of the pore structure and surface chemistry of the coal matrix.³⁰ Therefore, dual adsorption needs to be considered in order to properly explore the adsorption equilibrium of H₂O on coal. On this basis, an optimized BET model is needed to accurately fit the H₂O adsorption isotherm of coal.³¹ Therefore, the optimized BET model is given as follows

$$\frac{n^{\text{exp}}}{n_m} = \frac{K_1 \frac{P}{P_s}}{\left(1 - K_2 \frac{P}{P_s}\right) \left(K_2 \frac{P}{P_s} + K_1 \frac{P}{P_s}\right)} \quad (7)$$

$$n^{\text{exp}} = \frac{m_2 - m_1}{18 \times m_1} \quad (8)$$

Table 2. Experimental Data of Isothermal Adsorption of Water Vapor by Anthracite Coal

P/P_s	0	0.11	0.32	0.43	0.56	0.75	0.97
n (mmol/g)	0	0.4868	0.9788	1.1579	1.5278	2.0164	3.1253

where the contributions of the monolayer and multilayer adsorption sites to the adsorption capacity are given as follows

$$\frac{n_1}{n_m} = \frac{K_1 \frac{P}{P_s}}{1 - K_2 \frac{P}{P_s} + K_1 \frac{P}{P_s}} \quad (9)$$

$$\frac{n_2}{n_m} = \frac{K_1 K_2 \left(\frac{P}{P_s}\right)^2}{\left(1 - K_2 \frac{P}{P_s}\right) \left(1 - K_2 \frac{P}{P_s} + K_1 \frac{P}{P_s}\right)} \quad (10)$$

in which n^{exp} is the coal sample adsorption capacity for water vapor at P/P_s , mmol/g. n_1 and n_2 are the monolayer adsorption capacity and multilayer adsorption capacity at P/P_s , respectively, mmol/g. n_m is the maximum monolayer adsorption capacity, mmol/g. K_1 and K_2 are constant values related to monolayer and multilayer adsorption heat, respectively.

4. RESULTS AND DISCUSSION

4.1. Adsorption of Single Gases by Coal. The experimental data for the isothermal adsorption of water vapor by anthracite at different relative humidity values are shown in Table 2. The experimental data were fitted according to the optimized BET model, and the fitted curve is shown in Figure 2. The corresponding fitting parameters are shown in Table 3.

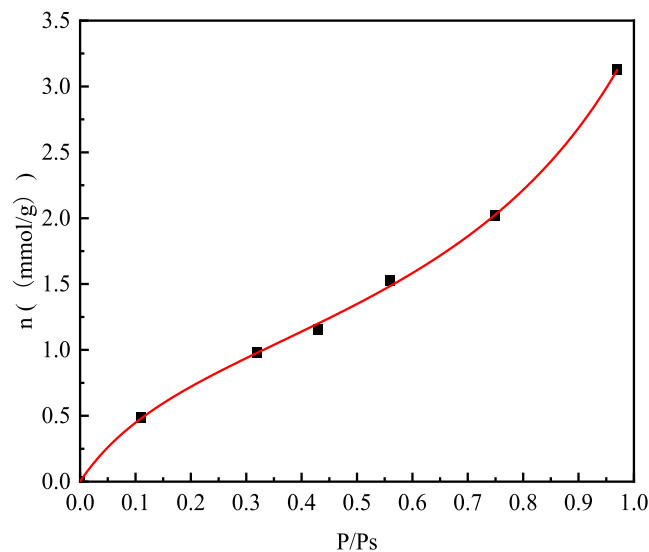


Figure 2. Fitting curve of the optimized BET model for water vapor adsorption on coal samples.

Table 3. Optimized BET Model Fitting Parameters

temperature (K)	n_m (mmol/g)	K_1	K_2	R^2
298.15	1.075	5.855	0.695	0.9991

According to Table 3, the coefficient of determination R^2 of the fitted curve is 0.9991, indicating that the improved BET model can well describe the adsorption equilibrium behavior of coal on water. According to previous research, the water vapor adsorption of coal comprises four different steps, which are

characterized as follows:²⁰ H₂O molecules are adsorbed on oxygen-containing functional groups as the main adsorption sites of the coal matrix (stage 1); H₂O molecules adsorbed by oxygen-containing functional groups in the coal matrix become adsorption sites for other H₂O molecules (stage 2); H₂O molecules gather to form clusters (stage 3); and micropore filling or capillary condensation of H₂O molecules occur in the pore space of coal (stage 4). In this case, monolayer adsorption usually occurs in stage 1 and multilayer adsorption occurs in stages 2–4. According to Figure 2, when $P/P_s < 0.56$, the adsorption of H₂O molecules is slower in stages 1–2, and when $P/P_s > 0.56$, the adsorption of the coal sample on water starts to rise steeply in stages 3–4 instead. There is a turning point at $P/P_s = 0.56$.

The experimental data for the isothermal adsorption of CH₄ and N₂ by anthracite in different moisture phases were fitted according to the Langmuir equation, and the fitted curves are shown in Figure 3. The isothermal adsorption constants “ a ” for CH₄ and N₂ were simulated by the Langmuir equation, and the terminal adsorption capacity was represented by “ a ”. The saturation adsorption capacities of the coal samples under the influence of different moisture phases are shown in Table 4.

From Figure 3, it can be seen that the adsorption capacity of CH₄/N₂ was greater in the coal samples treated with water vapor than in the coal samples treated with stirring. In addition, the difference in the adsorption capacity of CH₄/N₂ was greater for the coal sample with a 2.75% moisture content than for the sample with a 5.63% moisture content. From Table 4, it can be observed that at a moisture content of 2.75%, the difference between the saturation adsorption capacity of CH₄/N₂ for the coal samples treated with water vapor and those treated with liquid-phase water was 0.204/0.189 (cm³/g). At a moisture content of 5.63%, the difference between the saturation adsorption capacity of CH₄/N₂ for the coal samples treated with water vapor and those treated with liquid-phase water was 0.151/0.139 (cm³/g). It appears more clearly that there is a difference in the isothermal adsorption of the coal samples treated with different moisture phases.

This phenomenon can be attributed to the distribution of different moisture phases in the coal samples. Although both gas-phase water and liquid-phase water can enter the interior of the coal matrix, the gas-phase water is adsorbed on the adsorption sites where the moisture content is low and the adsorption sites are occupied, resulting in a decrease in the gas adsorption capacity. Compared with gas-phase water, liquid-phase water is easily formed by microporous filling or capillary condensation due to its nonuniform distribution in the coal matrix, resulting in a lower gas adsorption capacity of the coal sample.

4.2. Displacement Effects of Coal under the Influence of Different Moisture Phases. In order to analyze the influence of different moisture phases on the displacement of the coal samples, the experiments of N₂ injection to displace CH₄ in the coal samples treated with different moisture phases were carried out at 0.74 MPa, and the gas adsorption capacity of each gas after the displacement equilibrium is shown in Figure 4.

According to Figure 4, variations in the moisture content within the coal samples have a significant impact on the CH₄

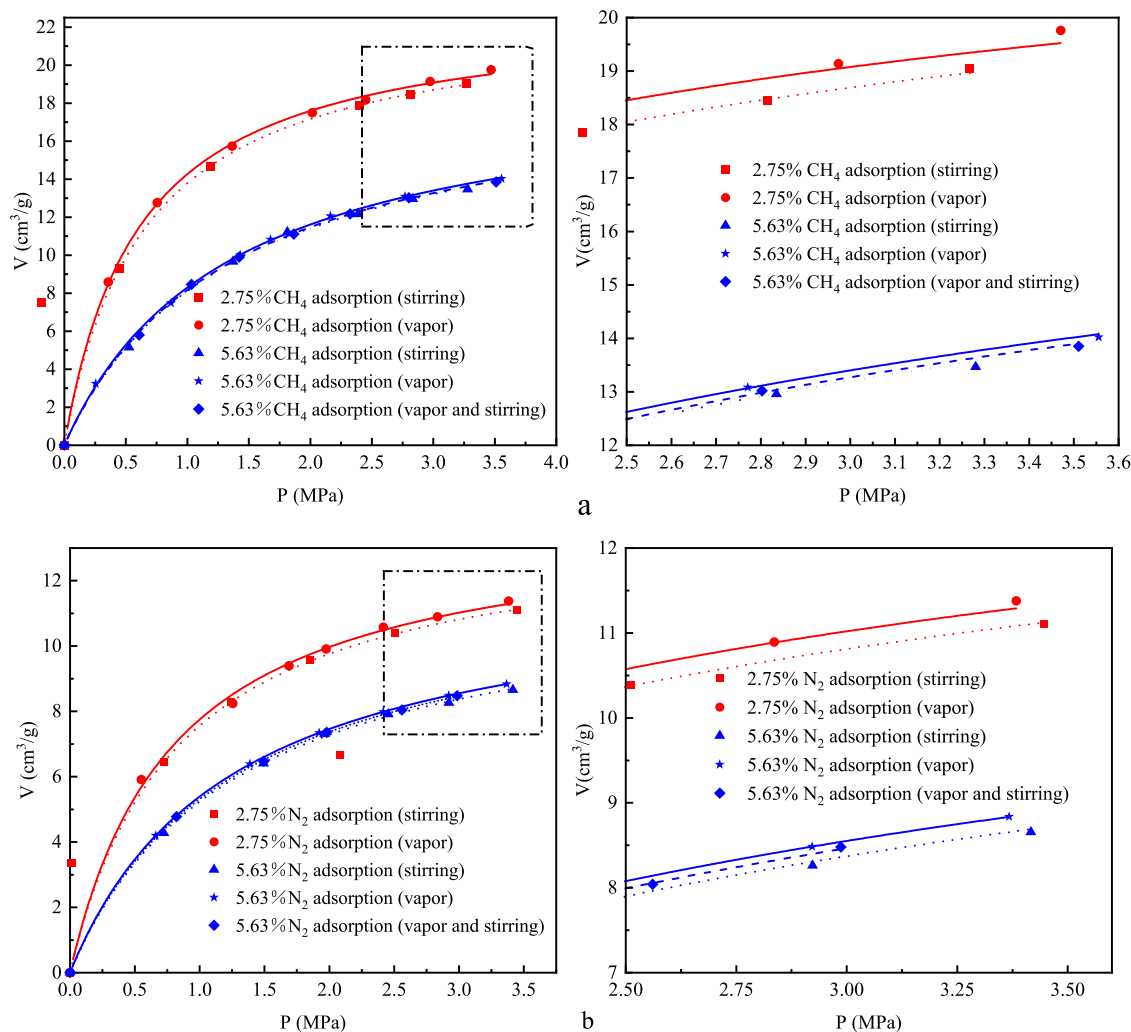


Figure 3. Isothermal adsorption capacities of CH₄ (a) and N₂ (b) on coals with different moisture phases and moisture contents after fitting the Langmuir equation.

Table 4. Saturation Adsorption Capacity of Coal Samples Treated with Different Moisture Phases

saturation adsorption capacities	CH ₄ (cm ³ /g)		N ₂ (cm ³ /g)	
	2.75%	5.63%	2.75%	5.63%
water vapor adsorption method	22.952	19.361	13.967	12.098
stirring method	22.748	19.210	13.778	11.959
water vapor adsorption and stirring method		19.307		12.022

adsorption capacity after displacement as well as the overall adsorption capacity of both N₂ and CH₄. In addition, at the same moisture content, there are disparities in the capacity of the displacement of CH₄ in coal by N₂ for the coal samples treated with different moisture phases. It is evident that the water-containing coal samples treated with water vapor adsorption exhibit higher total adsorption capacity, CH₄ adsorption capacity, and N₂ adsorption capacity after displacement than those treated with the stirring method. Moreover, at a moisture content of 2.75%, the disparity of total gas adsorption capacity is 0.62 cm³/g and that of CH₄ adsorption capacity is 0.473 cm³/g for the coal samples treated with different moisture phases. At a moisture content of 5.63%, the disparity of total gas adsorption capacity is 0.3 cm³/g and that of CH₄ adsorption capacity is 0.22 cm³/g for the coal samples treated with different moisture

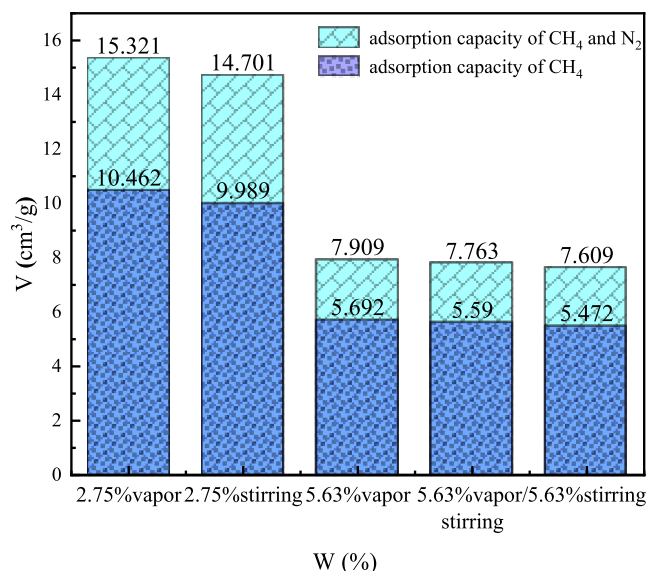


Figure 4. Gas adsorption capacity after displacement in different moisture phases.

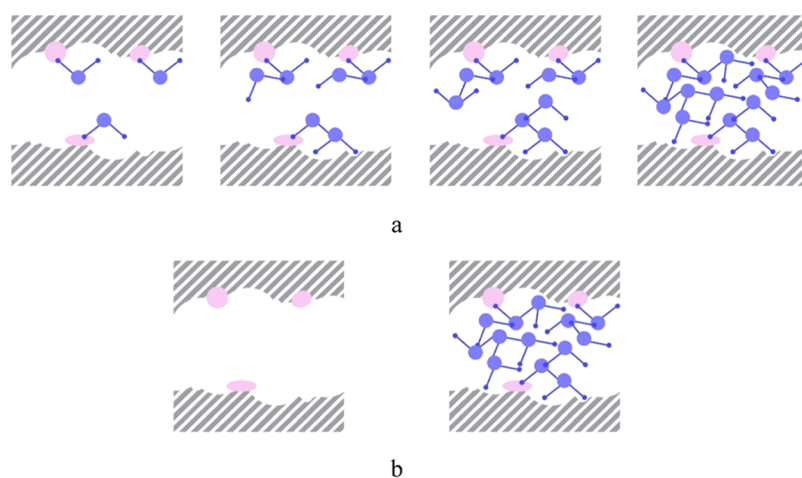


Figure 5. Different moisture phase adsorption steps: (a) water vapor adsorption by the coal sample and (b) liquid-phase water adsorption by the coal sample.

phases. The disparity in the adsorption capacity of the coal samples treated with different moisture phases is greater for a moisture content of 2.75% than for 5.63%.

The reason for this phenomenon is the different adsorption processes of the different moisture phases on the coal matrix; the different moisture phase adsorption steps are shown in Figure 5. According to the previous section, the adsorption of H₂O from the coal samples treated with water vapor adsorption has four variation processes with increasing moisture content. The gases are hindered from entering the pore interior in these processes; thus, the adsorption and diffusion of CH₄ and N₂ in the pores are affected. Conversely, in the case of the coal samples treated with the stirring method, ensuring uniform moisture distribution within the coal is a challenge. When a coal sample adsorbs liquid-phase water, the liquid-phase water enters the pores to form micropore filling or capillary condensation, which influences gas transport in the pores. This difference was statistically significant. At a moisture content of 2.75% ($P/P_s = 0.56$), the water vapor adsorption steps of the coal sample treated with the water vapor adsorption method are in stage 2. At a water content of 5.63% ($P/P_s = 0.97$), the water vapor adsorption steps of the coal sample are in stage 4. Therefore, the disparity in the adsorption capacity of the coal samples treated with different moisture phases is greater for a moisture content of 2.75% than for 5.63%.

In order to further explore the influence of different moisture phases on displacement, it is very necessary to study the CH₄ desorption capacity and desorption rate in the coal samples treated with different moisture phases. The formulation of the CH₄ desorption capacity and desorption rate is as follows

$$\Delta Q = Q_{x0} - Q_{x1} \quad (11)$$

$$\eta = \frac{\Delta Q}{Q_{x0}} \quad (12)$$

where ΔQ is the CH₄ desorption capacity after the gas injection displacement adsorption equilibrium, cm³/g. η is the desorption rate of CH₄. Q_{x0} is the adsorption capacity of CH₄ in coal before the gas injection displacement experiment, cm³/g. Q_{x1} is the adsorption capacity of CH₄ in coal after the adsorption equilibrium of gas injection displacement experiments, cm³/g.

The experimental results of the CH₄ desorption capacity and desorption rate in the experiments of N₂ displacement of CH₄ in

coal treated with different moisture phases are shown in Figures 6 and 7, respectively.

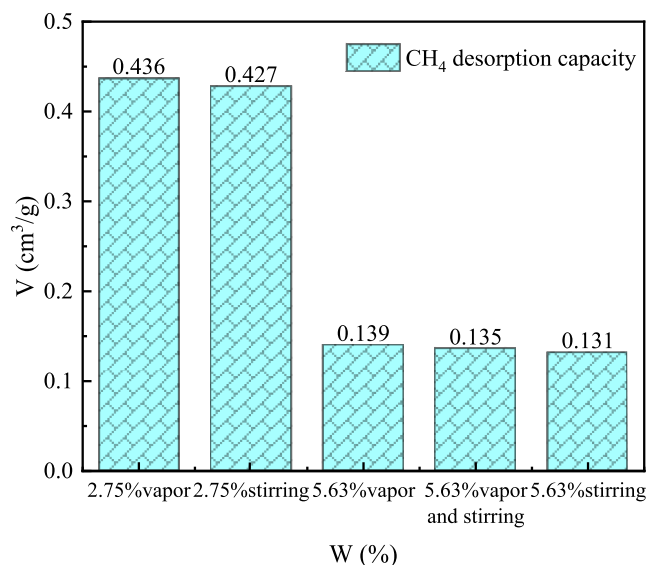


Figure 6. CH₄ desorption capacity at different moisture phases.

According to Figures 6 and 7, the desorption capacity and desorption rate of CH₄ from the water-containing coal samples treated with water vapor adsorption and stirring exhibit differences under equivalent moisture levels. In general, the desorption capacity and desorption rate of the samples treated with water vapor adsorption tend to be higher than those treated with liquid water. However, the differences were not significant. The reason for this is that the ability of N₂ to displace CH₄ is not powerful, and coupled with the influence of moisture content, the desorption capacity and rate are greatly affected; therefore, the differences in the influence of the moisture phases on the desorption capacity and rate are even smaller. Therefore, it is important to select different moisture phases in future experiments based on the specific experimental requirements to achieve a specific experimental purpose. In engineering practice, methane desorption is minimally affected by different moisture phases, so the impact of moisture phases on methane desorption on the injection of N₂ can be disregarded.

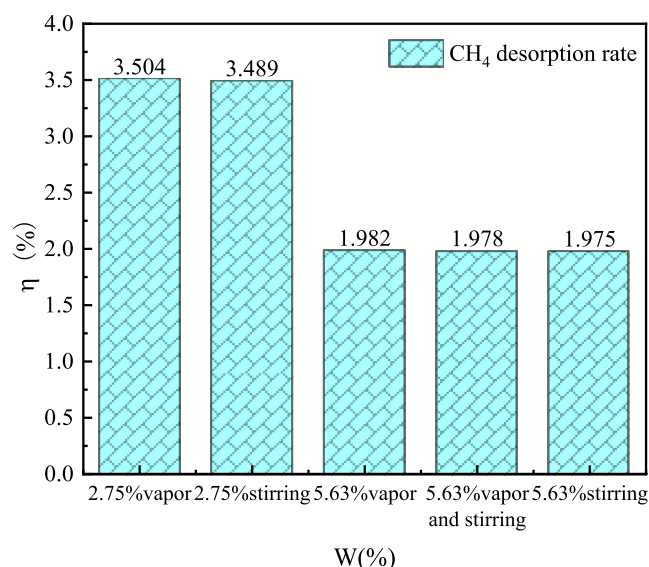


Figure 7. CH₄ desorption rate at different moisture phases.

5. CONCLUSIONS

There was a difference in the isothermal adsorption characteristics and displacement effect of the coal samples after treatment with different moisture phases. The main conclusions are as follows:

- (1) At the same moisture content, due to the different adsorption processes of coal to different moisture phases, the gas-phase water-treated coal sample exhibits higher isothermal adsorption capacities for CH₄/N₂ and higher CH₄ adsorption capacity, N₂ adsorption capacity, and total adsorption capacity after the displacement process compared to the liquid-phase water-treated coal sample.
- (2) At a moisture content of 2.75%, the difference between the saturation adsorption capacities of CH₄/N₂ for the coal samples treated with water vapor and those treated with liquid-phase water was 0.204/0.189 (cm³/g). At a moisture content of 5.63%, the difference between the saturation adsorption capacities of CH₄/N₂ for the coal samples treated with water vapor and those treated with liquid-phase water was 0.151/0.139 (cm³/g). At a moisture content of 5.63%, the difference in the isothermal gas adsorption for the coal samples treated with different moisture phases was higher.
- (3) In the displacement experiment, at a moisture content of 2.75%, the disparity of the total gas adsorption capacity is 0.62 cm³/g and that of the CH₄ adsorption capacity is 0.473 cm³/g for the coal samples treated with different moisture phases. At a moisture content of 5.63%, the disparity of the total gas adsorption capacity is 0.3 cm³/g and that of the CH₄ adsorption capacity is 0.22 cm³/g for the coal samples treated with different moisture phases.
- (4) At equivalent moisture levels, the differences in the moisture phases had minimal effects on the desorption capacities and rates of both CH₄ and N₂. For future laboratory experiments and field applications, the choice of the moisture phase should be tailored based on the specific requirements of the experiments and engineering practices to achieve the desired and cost-effective objectives.

In this article, experiments on the isothermal adsorption of CH₄/N₂ and N₂ displacement of CH₄ in the coal samples treated with different moisture phases were conducted, and the results showed that the isothermal adsorption characteristics and displacement effects of the coal samples were different for different various moisture phases. The adsorption and displacement processes of gases and different moisture phases in the coal matrix are complicated and difficult to observe step by step with experimental equipment and need to be further investigated in the future.

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Notes

The authors declare no competing financial interest.

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