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**Research Article**

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# Evaluation of Adsorption Models for Methane and Carbon Dioxide on Coal of Different Ranks

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**Abstract:** To evaluate the adsorption capacities of methane and carbon dioxide in coals of different ranks, the relationship between the adsorption amount and equilibrium adsorption pressure, as measured by the adsorption test apparatus, was analyzed. The equilibrium adsorption pressure was divided into small pressure intervals, and the adsorption amounts were non-linearly fitted using adsorption models such as Langmuir. By comparing the fitting accuracies of various adsorption models, the optimal adsorption model for different coal ranks in different pressure ranges was determined. The results show that the fitting accuracy of each model varies in different pressure intervals, demonstrating different applicability in different pressure ranges.

**Keywords:** Coal; Methane; Carbon Dioxide; Adsorption Models; Applicability.

## 1. Introduction

Methane and carbon dioxide are important gases in coalbed methane extraction and carbon dioxide capture fields. Their adsorption behavior directly impacts the gas storage capacity of coal reservoirs, the efficiency of coal gas extraction, and the storage and reduction effects of carbon dioxide [1]. Methane is a major component of natural gas, while carbon dioxide, as a greenhouse gas, causes significant climate change due to excessive emissions. Therefore, the adsorption of coalbed methane and the capture and sequestration of carbon dioxide have significant environmental and energy implications. The pore structure of coal, surface chemistry, and adsorption conditions affect gas adsorption capacity, and the differences in adsorption capacities of coals from different ranks make the evaluation of coal gas adsorption properties a complex issue [2].

In recent years, with the development of coalbed methane extraction technologies and the implementation of carbon dioxide reduction policies, both domestic and international research on methane and carbon dioxide adsorption in coal samples has deepened. Early studies focused on gas adsorption models that described single-layer adsorption, such as the Langmuir model, which assumes that the surface of the coal pores is uniform, with limited adsorption sites where each site can only adsorb one molecule [3]. However, as the pore structure of coal has been more thoroughly studied, an increasing number of studies have shown that the adsorption behavior of coal is not limited to single-layer adsorption, especially under high-pressure conditions, where gas molecules gradually enter deeper pores, forming multi-layer adsorption. Therefore, multi-layer adsorption models (such as the BET model, DA model, etc.) have gradually become the focus of research [4-9].

Although the Langmuir model performs well in low-pressure regions, its limitation lies in its ability to only describe single-layer adsorption and its difficulty in adapting to multi-layer adsorption in coal samples. To overcome this limitation, the BET model was introduced, which is based on the Langmuir model but assumes that gas molecules can form multiple adsorption layers on the adsorbent surface [10-14]. The BET model is particularly suitable for describing adsorption behavior at higher pressures, especially when gas concentrations are high. Furthermore, the DA model was introduced to describe the adsorption behavior of coal samples with heterogeneous surface properties. This model combines the advantages of the Langmuir model and, by

incorporating adsorption heat and pore structure factors, can more accurately predict adsorption characteristics in complex situations.

Internationally, research has shown that multi-layer adsorption models exhibit superior performance in describing the adsorption behavior of coalbed methane and carbon dioxide [15]. For example, Cohen et al. (2014) proposed that when predicting $CO_2$ adsorption using the BET model, it better simulates the adsorption characteristics of coalbed methane. Later, Sharma and Aggarwal (2016) further explored the applicability of multi-layer adsorption to different coal types and pointed out that under high pressure, the BET and DA models outperform the Langmuir model in predicting $CO_2$ adsorption. In addition, with the advancement of experimental technologies, more researchers have started using different adsorption models to analyze the adsorption performance of coals of different ranks. For example, Zhang et al. (2020) fitted methane adsorption data for coal samples of different ranks using the Langmuir, BET, and D-R equations, and compared the fitting accuracy of each model, proposing a method to select the best adsorption model for different pressure ranges.

Although many adsorption models have been proposed and applied to coal gas adsorption research, how to accurately select the best adsorption model for different coal samples and gases remains a challenge. Different adsorption models take into account different factors when describing the adsorption process, such as the uniformity of pore structure, variations in adsorption phase density, and the interactions between gas molecules, which leads to differences in their applicability under the same pressure range and different coal sample conditions. Therefore, fitting multiple models and comparing their fitting accuracy to choose the most suitable model for predicting adsorption behavior is of significant practical value for coalbed methane extraction and carbon dioxide reduction.

This study aims to compare and analyze different adsorption models, including Langmuir, BET, and DA models, to evaluate their applicability in coal samples of different ranks, especially in adsorption behavior under different pressure ranges [16]. By fitting experimental data, the strengths and weaknesses of each model in predicting methane and carbon dioxide adsorption are analyzed, and the best model is selected based on the fitting accuracy. This will not only help improve the understanding of gas adsorption characteristics in coal samples but also assist in optimizing coalbed methane extraction plans and improving carbon dioxide capture and sequestration efficiency.

## 2. Methane and Carbon Dioxide Absolute Adsorption Amount Correction

### Correction Research Status

Adsorption amount correction is the process of solving the relationship between adsorption amount and conditions such as pressure and temperature based on adsorption test data and certain physical models. Commonly used correction methods include adsorption phase density correction, Langmuir model, and BET model. These models can correct the raw adsorption amounts measured experimentally, thereby accurately predicting the adsorption behavior of different gases in coal samples [17].

A large body of previous research has conducted detailed analyses of methane and carbon dioxide adsorption correction methods, presenting various correction methods with their advantages, disadvantages, and applicable ranges. In their studies, adsorption amount correction based on the Langmuir model effectively describes adsorption behavior under low pressure, while correction based on the BET model is better suited for multi-layer adsorption, especially in medium to high pressure ranges [18].

### Methane and Carbon Dioxide Correction Methods

To more accurately evaluate the adsorption capacity of methane and carbon dioxide in coal, this study adopts correction methods based on the Langmuir and BET models. The Langmuir model is used to describe single-layer adsorption, while the BET model considers the case of multi-layer adsorption. By combining the experimentally measured adsorption amounts and pressure relationships, and incorporating adsorption phase density, the adsorption amount is optimized and corrected.

The specific correction formulas are as follows:

**i. Langmuir Model**

$$M_e = \frac{V_L \cdot P}{(P_L + P)} \cdot \left(1 - \frac{\rho_g}{\rho_a}\right)$$

In this case, $M_e$ represents the adsorption amount; $V_L$ is the adsorption amount when the adsorbent surface is covered by a monolayer; $P$ is the adsorption equilibrium pressure; $P_L$ is the Langmuir constant; $\rho_g$ is the gas density; and $\rho_a$ is the density of the adsorbed phase.

**ii. BET Model**

$$M_e = \frac{V_m \cdot C \cdot P}{(P_0 - P)} \cdot \left(1 - \frac{\rho_g}{\rho_a}\right)$$

In this case, $V_m$ represents the adsorption amount of a monolayer; $C$ is a constant related to the adsorption heat; and $P_0$ is the saturation vapor pressure of the gas.

**iii. D-A Model**

$$M_e = V_0 \cdot \exp\left[-D \cdot \ln\left(\frac{P_0}{P}\right)\right] \cdot \left(1 - \frac{\rho_g}{\rho_a}\right)$$

In this case, $V_0$ represents the maximum adsorption amount when the micropores are filled; $D$ is a constant related to the adsorption heat; and n is a dimensionless parameter related to the surface heterogeneity of the adsorbent.

## 3. Selection of the Best Model

**Model Introduction**

**Langmuir Model**

The Langmuir model is suitable for describing single-layer adsorption, assuming that the adsorption sites are homogeneous and each site can only adsorb one molecule. When the gas molecule concentration is low, the Langmuir model effectively describes the adsorption process [19]. However, its applicability decreases when high concentrations of gas are present.

**BET Model**

The BET model is suitable for multi-layer adsorption, taking into account the interaction between gas molecules and the impact of the pore structure of the coal sample on the adsorption process. When the gas concentration is high, and multi-layer adsorption dominates, the BET model more accurately reflects the adsorption process.

**DA Model**

The DA model combines the advantages of the Langmuir and BET models, and can describe more complex adsorption behaviors, particularly when the coal sample's pore structure is heterogeneous or when there are significant changes in adsorption phase density. The DA model performs more stably under these conditions.

**Model Fitting**

In practical applications, different adsorption models are used to fit the adsorption amount based on experimental data from different pressure intervals. By comparing the fitting accuracy, the best model is selected. Each model has different assumptions and applicable ranges, so it is necessary to choose the model based on the pore structure of the coal sample and the gas adsorption characteristics [20].

**Comparison of Fitting Accuracy for Model Selection**

The adsorption amount curve obtained from the fitting is compared with experimental data, and the fitting errors and correlation coefficients are calculated to determine which model has higher fitting accuracy. For different pressure ranges, it may be necessary to select different models to ensure the best description of the adsorption behavior. The higher the fitting accuracy, the stronger the model's applicability.

## 4. Conclusion

Through fitting and comparison of different adsorption models, it was found that the adsorption behavior of different coal samples varies in different pressure ranges. The Langmuir model performs better in the low-pressure range, while the BET and DA models are better suited to describe high-pressure and multilayer adsorption situations. Therefore, selecting the most suitable adsorption model not only depends on the characteristics of the coal sample but also needs to consider experimental conditions, gas properties, and the pressure range of adsorption. It is recommended to choose the appropriate model based on the pressure range and coal sample type in practical applications to obtain more accurate adsorption predictions.

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