Theoretical Derivation of a Prediction Model for CO₂ Adsorption by Coal

Jianchi Hao,* Hu Wen, Li Ma, Jinbiao Fei, and Lifeng Ren

ABSTRACT: Adsorption characteristics of CO₂ by coal are an important reservoir parameter to determine the CO₂ storage capacity of the coal seam. The Langmuir isotherm adsorption model is commonly used to describe the isothermal adsorption line of coal. However, we cannot predict the CO₂ adsorption capacity at other temperatures by using the Langmuir model based on the experimental data at a fixed temperature. This paper analyzes the ε−V₂ adsorption characteristic curves of three coal samples over a range of temperatures and pressures. The study demonstrates that the adsorption characteristic curves of CO₂ gas are independent of temperature and depend mainly on the dispersion force between coal and the CO₂ molecules. In addition, the adsorption potential of CO₂ gas has a negative correlation with the volume of the adsorbed phase. Hence, the CO₂ adsorption characteristic curve of coal conforms to the logarithmic function. Based on the adsorption potential theory, the prediction model of CO₂ adsorption by coal is derived. The deviation analysis from measured data shows that the average relative deviation of the three coal samples is ~5%, and the prediction results are accurate and reliable. Under different temperature and pressure conditions of the three coal samples, the results from the prediction model of CO₂ adsorption by coal and the Langmuir model have a strong correlation with the experimental results. In comparison with the Langmuir model, the prediction model of CO₂ adsorption by coal can predict the adsorption capacity under different temperature and pressure conditions. Hence, it has a wide range of applications when compared to that of the Langmuir model. In practical applications, better results are achieved with a significant reduction in experimental time and labor.

1. INTRODUCTION

Global temperature rise, glacier melting, rise in sea level, extinction of some species, ecological imbalance, the spread of infectious diseases, and other adverse effects caused by significant CO₂ emissions are some of the common worldwide problems.¹–³ In order to find viable solutions to these issues, various international agencies, climate organizations, and governments pursue fast and effective ways to reduce CO₂ emissions.⁴–⁵ At present, the main technologies for CO₂ emission reduction are the source control green clean energy technology, the process control fossil energy emission reduction technology, and the end control CO₂ capture and storage technology (CCS); of these, the green clean energy solution appears to be the most preferred option.⁶–¹² However, these green and clean energy technologies are still in the research stage and cannot replace fossil energy in the near future.¹²–¹⁵ By 2030, the International Energy Agency foresees fossil energy to be the main source of primary energy, accounting for 84% of the total energy demand growth.¹⁶ Therefore, the CCS technology is the most effective way to reduce CO₂ emissions.

The geological storage of CO₂ is a novel greenhouse gas storage technology. The CO₂ separated from the centralized emission source is injected deep into the underground and isolated in the stratum with appropriate sealing conditions.¹⁷,¹⁸ At present, the most studied underground storage methods of CO₂ for various applications are deep saline water storage, oil and gas field storage, and deep coal seam storage without a commercial exploitation value.¹⁹,²⁰ Among these storage options, the adsorption characteristics of CO₂ by coal are an important reservoir parameter to determine the CO₂ storage capacity of the coal seam. The Langmuir model is a popular method to study the isothermal adsorption line of CO₂. This model is simple, and its characteristic constants have clear physical significance, which has been confirmed by a large number of experiments.²¹–²³ Recent studies show that the limitation of the Langmuir isotherm adsorption model is that the
isothermal formula of CO₂ adsorption by coal can be obtained from experimental data only at a specific temperature. This model cannot predict the amount of CO₂ adsorption by coal under other temperature and pressure conditions. Therefore, using the Langmuir model to obtain the characteristic constants of CO₂ adsorption by coal requires time- and labor-intensive experiments.

Based on the above problems, a prediction model of CO₂ adsorption capacity is proposed by using the principle of adsorption potential. According to the experimental data at one temperature, the CO₂ adsorption capacity at other temperatures can be predicted, which can effectively shorten the cycle of the CO₂ adsorption experiment.

2. CO₂ GAS ISOTHERMAL ADSORPTION EXPERIMENT

Figure 1 shows the experimental setup using a high-pressure gas adsorption/desorption instrument, which is mainly composed of a coal sample container, pneumatic valve, gas storage tank, pressure control unit, temperature sensor, vacuum pump, and gas cylinder.

According to the metamorphic degree of different coals, the long flame coal, charred coal, and anthracite were selected as experimental coal samples. The industrial analysis of coal samples is shown in Table 1. First, the three coal samples are crushed to an 80 mesh and dried in a drying box at 80 °C. The dried samples were used in the isothermal adsorption experiments under different temperatures and pressures. The temperature range is ~30–60 °C, and the pressure range is ~0–5 MPa.

3. ADSORPTION CHARACTERISTIC CURVES OF COAL TO CO₂

Polanyi’s adsorption potential theory states that the adsorption potential of an adsorbate molecule in the field of attraction on a solid surface is the work required to move the molecule from its position to infinity in the adsorption space. Therefore, the adsorption potential theory reflects the change law of Gibbs free energy when the adsorbent adsorbs unit molar mass of the adsorbate. In this theory, the pressure at which the ideal gas is adsorbed is assumed to be \( P_i \) and the pressure of the adsorption layer on the solid surface is equal to the saturated vapor pressure of the adsorbed gas \( P_0 \). According to the thermodynamic molecular adsorption theory, the work in transferring the mass per unit mass of the adsorbate from the free state of the non-adsorbed phase to the adsorbed state of the adsorbed phase is assumed to be \( \epsilon \). It can be expressed as

\[
\epsilon = \int_{P_i}^{P_0} \frac{RT}{P} \, dP = RT \ln \frac{P_0}{P_i}
\]

In eq 1, \( \epsilon \) is the adsorption potential (J/mol), \( P_0 \) is the gas saturated vapor pressure (MPa), \( P_i \) is the equilibrium pressure of the ideal gas at constant temperature (MPa), \( R \) is the universal gas constant [J/(mol·K)], and \( T \) is the absolute temperature (K).

In practical applications, the ambient temperature of CO₂ adsorption by coal is always above its critical temperature. Therefore, the saturated steam pressure \( (P_0) \) under critical conditions is calculated using the empirical calculation formula of virtually saturated steam pressure under supercritical conditions proposed by Dubinin:

\[
P_0 = P_c \left( \frac{T_c}{T} \right)^2
\]

Table 1. Industrial Analysis of Coal Samples

| coal sample  | moisture/% | ash/% | volatile matter/% |
|--------------|------------|-------|-------------------|
| long flame coal | 5.58 | 12.37 | 42.28 |
| charred coal   | 5.52 | 6.29  | 44.48 |
| anthracite coal| 1.86 | 9.97  | 36.35 |

\( P_0 \) is the critical pressure of the gas (MPa), and \( T_c \) is the critical temperature of the gas (K). In this study, the \( T_c \) of CO₂ is 304.2 K and the \( P_c \) of CO₂ is 7.39 MPa.

Physical adsorption works mainly by dispersion force and is independent of temperature. Therefore, it can be concluded that the relationship between adsorption potential and adsorption phase volume in the same adsorption system will not be affected by temperature. In other words, the \( \epsilon = V_{ad} \) relationship of an adsorbent to a given gas should be unique, and this is called the adsorption characteristic curve. The volume of the adsorbed phase can be obtained from eq 3:

\[
V_{ad} = \frac{m}{\rho_{ad}} = \frac{V \times 44}{22,400 \times \rho_{ad}}
\]
Here, $V_{ad}$ is the volume of the adsorption phase under equilibrium conditions (cm$^3$/g), $V$ is the adsorption amount of the gas under equilibrium condition (cm$^3$/g), $m$ is the mass of the adsorbed gas (g), $\rho_{ad}$ is the density of the adsorption phase (g/cm$^3$), and the adsorption phase density of CO$_2$ is 1.023 g/cm$^3$.

According to the isothermal adsorption experimental data, the CO$_2$ adsorption potential $\varepsilon$ and the adsorption phase volume $V_{ad}$ of each coal sample under different temperature conditions were calculated, and the CO$_2$ gas adsorption characteristic curves of coal are shown in Figures 2–4.

It can be seen from Figures 2–4 that the $\varepsilon$–$V_{ad}$ characteristic curves of the three coal samples of different coal grades at different temperatures almost fall on the same curve. This indicates that the $\varepsilon$–$V_{ad}$ characteristic curve is independent of temperature, and as the dispersion force plays a major role between coal and CO$_2$ gas molecules, the adsorption process of coal to CO$_2$ gas is by physical adsorption. Similarly, it is observed that the adsorption potential of CO$_2$ gas has a negative correlation with the volume of the adsorbed phase, and the expression used is $\varepsilon = a \times \ln(b \times V_{ad})$. The correlation coefficients of long flame coal, charred coal, and anthracite coal are 0.96167, 0.94888, and 0.94085, respectively. It can be concluded that the CO$_2$ adsorption characteristic curve of coal conforms to the logarithmic function.

4. DERIVATION OF THE PREDICTION MODEL FOR CO$_2$ ADSORPTION BY COAL

As the volume $V_{ad}$ of the CO$_2$ adsorbed phase of coal has a linear relationship with the adsorption capacity $V$

$$V_{ad} = \frac{m}{\rho_{ad}} = \frac{V \times 44}{22,400 \times \rho_{ad}}$$

(4)

where $V_{ad}$ is the volume of the adsorbed phase under equilibrium conditions (cm$^3$/g), $V$ is the adsorption capacity of the gas under equilibrium conditions (cm$^3$/g), $m$ is the mass of the adsorbed gas (g), $\rho_{ad}$ is the density of the adsorption phase (g/cm$^3$), and the adsorption phase density of CO$_2$ is 1.023 g/cm$^3$.

It can be seen that there is also a logarithmic function relationship between the adsorption potential $\varepsilon$ and the adsorption capacity $V$ of CO$_2$, that is, $\varepsilon = a \times \ln(b \times V_{ad})$.

$$\varepsilon = a \times \ln(b \times V_{ad})$$

(5)

$$\varepsilon = c \times \ln(d \times V)$$

(6)

Incorporating these values in eq 6 gives

$$\ln V = \frac{\varepsilon}{c} - \ln d$$

(7)

$$V = e^{\varepsilon/c} \times \frac{d}{\varepsilon}$$

(8)

Since $C$ and $D$ are constants, let $C = \frac{1}{c}$ and $D = \frac{1}{d}$ be constant. Then,

$$V = D \times e^{C\varepsilon}$$

(9)

If $a$ is introduced into eq 9, then
\[ V = D \times e^{\frac{CRT}{T}} \ln p / p \]  
(10)

Substituting \( p_0 = \frac{T_e}{T} \cdot \frac{p}{p_0} \) into eq 10, we get
\[ V = D \times e^{\frac{CRT}{T}} \ln p / p_0 \]  
(11)

In Equation 11, \( V \) is the CO2 adsorption capacity \( (\text{cm}^3/\text{g}) \), \( T \) is the equilibrium temperature \( (\text{K}) \), \( P \) is the equilibrium pressure of CO2 gas \( (\text{MPa}) \), \( P_0 \) is the Dublin pseudo-saturated vapor pressure \( (\text{MPa}) \), and \( R \) is the gas constant.

In order to calculate the characteristic constants \( C \) and \( D \) in the model, the natural logarithm of eq 11 is used to yield the following equation
\[
\ln V = \ln(D e^{CRT \ln p / p}) = \ln D + CRT(\ln p_0 - \ln p)
\]
\[
= \ln D + CRT \ln p_0 - CRT \ln p = \ln D + CRT\n\]
\[
\ln\left[p_0 \left(\frac{T}{T_e}\right)^2\right] - CRT \ln p = \ln D
\]
\[
+ CRT[\ln p + 2(\ln T - \ln T_e)] - CRT \ln p
\]  
(12)

Let
\[ a = CRT \]  
(13)
\[ b = \ln D + CRT[\ln p + 2(\ln T - \ln T_e)] \]  
(14)

Then, eq 12 becomes
\[ \ln V = b - a \ln p \]  
(15)

where \( a \) and \( b \) are undetermined coefficients. Here, \( T_e \) is the critical temperature of the gas \( (\text{K}) \). The \( T_e \) of CO2 is 304.2 K, and the critical pressure \( P_c \) is 7.39 MPa.

In each coal sample, \( a \) and \( b \) are calculated as follows:

(1) The natural logarithmic values of \( \ln V \) and \( p \) for different values of equilibrium pressure and the corresponding adsorption capacities are calculated based on the isothermal adsorption test results of samples at a certain temperature;

(2) Using the calculated \( \ln V \) and \( p \) values in the direct coordinate system, the correlation formula \( \ln V = b - a \ln p \) and the undetermined coefficients \( a \) and \( b \) are obtained;

(3) The values of \( a \) and \( b \) are substituted into eqs 13 and 14, respectively, and the characteristic constants \( C \) and \( D \) of the adsorption model of each coal sample at this temperature are calculated
\[ C = \frac{a}{RT} \]  
(16)
\[ D = e^{b-a[\ln p + 2(\ln T - \ln T_e)]} \]  
(17)

(4) The specific prediction model of CO2 adsorption by coal was obtained by substituting the values of \( C \) and \( D \) into eq 10, and the adsorption capacity of coal to CO2 gas was calculated under different pressure and temperature conditions.

5. VALIDATION OF THE PREDICTION MODEL FOR CO2 ADSORPTION BY COAL

Isothermal adsorption experiments were carried out on the three samples of long flame coal, charred coal, and anthracite coal at 30 °C. According to the aforementioned model, the undetermined coefficients \( a \) and \( b \) in the logarithmic relationship between the measured adsorption capacity and the experimental equilibrium pressure of each coal sample at this temperature were obtained. Figure 5 shows the \( \ln V - \ln p \) fitting curve, and the prediction model of CO2 adsorption of each sample at this temperature was calculated. The characteristic constants \( C \) and \( D \) are shown in Table 2.

| coal sample          | fitting \( \ln V - \ln p \) equation by the isothermal adsorption experiment at 30 °C | \( R^2 \)      | \( C \)         | \( D \)         |
|----------------------|------------------------------------------------------------------------------------------|----------------|----------------|----------------|
| long flame coal      | \( \ln V = 3.04749 + 0.58039 \ln p \)                                                    | 0.99209        | -0.0002304     | 254.8634       |
| charred coal         | \( \ln V = 3.44375 + 0.54257 \ln p \)                                                    | 0.99607        | -0.0002154     | 321.9901       |
| anthracite coal      | \( \ln V = 4.43805 + 0.37064 \ln p \)                                                    | 0.99399        | -0.0001471     | 415.8166       |

The calculated characteristic constants are substituted into eq 10 to obtain the predicted adsorption amount of CO2 gas under each experimental equilibrium pressure of 40, 50, and 60 °C. The results are shown in Figures 6–8.

It can be seen that the predicted adsorption capacity of coal at 40, 50, and 60 °C is very close to that of each equilibrium pressure point measured by the experiment, and the change trend is consistent. The adsorption amount of CO2 by coal decreases with an increase in temperature.

In order to analyze the difference between the adsorption amount from the prediction model and the experiment, the absolute deviation, relative deviation, and average relative deviation are used for the different analyses.

Absolute deviation = predicted adsorption amount – experimental adsorption amount

Relative deviation = absolute deviation/experimental adsorption amount

The average deviation refers to the arithmetic mean of the relative deviation of the sample under various equilibrium pressures at a specific temperature.
The absolute deviation, relative deviation, and average deviation between the predicted adsorption capacity and the experimentally measured adsorption capacity of each coal sample under different temperatures and experimental equilibrium pressures were calculated. Figures 9–11 show the deviation analysis between the predicted data and the experimental data of 98 pressure points at 40, 50, and 60 °C.

It can be seen from Figures 9–11 that the absolute deviation between the adsorption capacity calculated by the CO₂ adsorption prediction model and the measured adsorption capacity in the isothermal adsorption experiment under the corresponding conditions is < 10 cm³/g, accounting for ~80%. The relative deviation <5 and 10% accounted for 59.18 and 84.69%, respectively. The average relative deviations of anthracite coal at 40 and 50 °C are 7.97 and 7.78%, respectively. The average relative deviation of other coal samples is ~5% at 40–60 °C. The possible reasons why the average relative deviation of anthracite is slightly higher than that of other coal samples are as follows: (1) the heterogeneity of coal surface. Because the assumption of this model is that the adsorption surface has the same adsorption capacity, but for coal, the properties of different components and different pore fissure surfaces are different, there will be some errors. (2) For the adsorption form of CO₂ on the coal surface, the assumption of this model is monolayer adsorption, but the actual adsorption situation may not be consistent with it. Monolayer adsorption may be the main adsorption form, but there are a small number of other adsorption forms, so the average relative deviations are formed.

In order to better explain the applicability of the prediction model for CO₂ adsorption by coal, the correlation analysis was carried out between the measured adsorption amount at each equilibrium pressure point of the three coal samples at different temperatures and the established prediction model of CO₂ adsorption by coal. The results of the correlation analysis are shown in Table 3.
It can be seen that there is a good correlation between the predicted adsorption amount and the measured adsorption amount of the three coal samples, and the correlation coefficient $R^2$ value > 0.99. It can be seen that the prediction model of CO$_2$ adsorption by coal is verified by the measured data from the isothermal adsorption experiment, and the prediction results are accurate and reliable.

### 6. COMPARISON BETWEEN THE PREDICTION MODEL AND THE LANGMUIR MODEL OF CO$_2$ ADSORPTION BY COAL

The classic Langmuir isotherm adsorption model is used to study the adsorption of CO$_2$ by coal. Therefore, from the results of the isothermal adsorption experiments of long flame coal, charred coal, and anthracite coal at 40 °C, the adsorption capacities of coal adsorption of CO$_2$ from the prediction model and Langmuir model were calculated under different equilibrium pressures, and the isotherms were plotted. Similarly, the correlation between the CO$_2$ adsorption by coal from the prediction model and Langmuir model and the measured data from the isothermal experiment was calculated and compared. The comparison results are shown in Figures 12–14 and Table 4.

Table 4 demonstrates that the prediction data of coal adsorption of the CO$_2$ model and Langmuir model have a good correlation with experimental data, and the correlation of...
coal adsorption of the CO₂ prediction model is better than that of the Langmuir model. Figure 8 shows that the predicted adsorption amount of CO₂ by coal is similar to that predicted by the Langmuir model, which closely matches the experimental adsorption amount.

Also, it can be seen from the Langmuir model equation (18) that the only variable is the equilibrium pressure \( P \), which predicts the adsorption capacity at each equilibrium pressure point at a specific temperature. Equation 10, obtained by the prediction model for CO₂ adsorption by coal, contains not only pressure \( P \) but also the temperature \( T \) term and can predict the CO₂ adsorption capacity at different temperatures and different equilibrium pressure points. From this point of view, the applicability of the coal adsorption CO₂ prediction model discussed in this paper has a wider scope than that of the Langmuir prediction model. In practical applications, it can substantially reduce experimental time and labor to yield better results.

\[
V = \frac{abp}{1 + bp} \tag{18}
\]

In eq 18, \( V \) is the adsorption capacity at equilibrium pressure \( p \) (cm³/g); \( a \) is the maximum adsorption capacity of the coal sample (cm³/g); and \( b \) represents the comprehensive parameters of adsorption, desorption speed, and adsorption heat.

In order to verify the CO₂ adsorption prediction model better, we calculated the adsorption potential by using the adsorption capacity predicted by the CO₂ adsorption prediction model and Langmuir model, respectively. The calculated results are compared with the experimental data. The results are shown in Figure 15.

7. CONCLUSIONS

(1) The \( \varepsilon - V_{ad} \) characteristic curves of the three coal samples of different coal grades at different temperatures are analyzed. It can be concluded that the \( \varepsilon - V_{ad} \) characteristic curves are independent of temperature, and as the dispersion force plays a major role between the coal and CO₂ gas molecules, the adsorption process of coal to CO₂ gas is by physical adsorption. At the same time, the adsorption potential of CO₂ gas has a negative correlation with the volume of the adsorbed phase. \( \varepsilon = a \times \ln(b \times V_{ad}) \). Thus, the CO₂ adsorption characteristic curve of coal conforms to the logarithmic function, and the expression is \( \varepsilon = a \times \ln(b \times V_{ad}) \).

(2) Based on the adsorption potential theory, the prediction model of CO₂ adsorption by coal was derived. The relationship between the adsorption capacity and temperature and pressure was obtained by \( V = D \times e^{CRT \ln T / R T^2} \) and verified by isothermal experimental data. The predicted adsorption amount of the three coal samples had a good correlation with the measured adsorption amount, and the correlation coefficient \( R^2 \) value was >0.99. The deviation analysis between the predicted adsorption capacity and the
measured adsorption capacity shows that the absolute deviation is <5 cm³/g, accounting for 66.33%, and the relative deviation <10% is ~85%. The average relative deviation of coal samples at ~40–60 °C is ~5%. The prediction results are accurate and reliable.

(3) It can be concluded that the predicted adsorption amount of CO₂ by coal is almost the same as that predicted by the Langmuir model, which is close to the experimental adsorption amount. However, the established prediction model of CO₂ adsorption by coal can predict the adsorption capacity under different temperature and pressure conditions. Hence, it has a wide range of applications when compared to the Langmuir prediction model. In practical applications, better results are achieved with a significant reduction in experimental time and labor.

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