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Study on the relationship between adsorption amounts and unit isosteric adsorption enthalpy

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Abstract: The isothermal adsorption data of a lean coal has been used to regress the parameters of a temperature-pressure-adsorption equation with acceptable accuracy. The lnP vs 1/T plotting of lean coal under 15 cm^3/g isosteric adsorption indicates that the adsorption is an exothermic process, the desorption is an endothermic process. Both the unit isosteric adsorption enthalpy (UIAE) and the unit isosteric desorption enthalpy (UIDE) have been calculated for different capacities and show that both UIAE and UIDE decrease with the increase of capacity.

Keywords: The isothermal adsorption; temperature-pressure-adsorption equation; unit isosteric adsorption enthalpy; unit isosteric desorption enthalpy.

I. INTRODUCTION

Coal's adsorption and desorption coexist with coal and gas outburst disasters. They are influenced by each other. Many studies compare the isothermal adsorption [1, 2] of different coals, the mathematical model and empirical formula of gas emission and desorption [3, 4], the difference in pore structure characteristics [5, 6], the change of coal temperature and the connection between coal and gas outburst [7, 8]. Chemical thermodynamics is the study of, from the perspective of energy, the substance regarding the questions, such as "In what state is the substance most stable?", "What product's energy is the lowest?", and "What is the direction of the chemical reaction, and the degree that can be achieved?". These theoretical hypotheses all agree to varying degrees: the coal and gas outburst process is accompanied by a repeating process of outside environmental energy transfer into the system and the internal energy accumulation and redistribution until the coal and gas outburst happening. This paper will discuss the thermodynamic calculation of internal energy transferring, accumulating, and redistributing with real tested data of a lean coal sample.

II. ISOTHERMAL ADSORPTION DATA TRANSFORMATION

A. Isothermal adsorption

The isothermal experimental temperatures of the lean coal were 293 K to 333 K, and the pressure range was up to 10 MPa. The isothermal adsorption data are listed in Table 1.

TABLE 1: THE ISOTHERMAL ADSORPTION DATA OF LEAN COAL [8]

Temperature	a	b
293K	45.27	0.383
303K	41.47	0.351
313K	40.04	0.317
323K	40.38	0.257

Where:
a is the Langmuir volume, cm^3/g.
b is the reciprocal of the Langmuir pressure, MPa^{-1}.

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B. Temperature-Pressure-Adsorption Equation [9-11]

Using the temperature and pressure as independent variables and adsorption amount as dependent variable, the temperature-pressure-absorbing equation can be expressed as

$$V = \frac{1}{\sqrt{MT}}\left[A + BP^{\beta}T^{1.5}\exp\left(\frac{\Delta}{T}\right)\right] \tag{1}$$

Where:

A is a constant of microporous geometric shape for a fixed porous medium, dimensionless.
B is the adsorption flow coefficient, which is related to the adsorption area, dimensionless.
M is a molecular weight, and the molecular weight of methane is 16.
V is the adsorption amount (cm^3/g).
b is a parameter which measures the relative influence of adsorption pressure, dimensionless.
Δ is the energy difference between the lowest potential energy and the activation energy of an adsorbed molecule in the adsorbed mass flow, which mainly measures the relative influence of the adsorption temperature, K.

The details regarding the regression of TPAE from series Longmuir adsorption has been presented early. The four parameters of TPAE regressed from Table 1 parameters of normal coal and deformed coal are listed in Table 2.

TABLE 2: THE TPAE PARAMETERS REGRETTED FROM ISOTHERMAL ADSORPTION MEASUREMENTS OF NORMAL COAL AND DEFORMED COAL

Parameter	Lean coal
A	0.168
B	0.00323
D/K	1173
b	0.4819

Since the TPAE is a mathematical expression of temperature-pressure-adsorption, TPAE could be presented in a three-dimensional picture as shown in Figure 1. TPAE treats accurately series isothermal adsorption of lean coal.

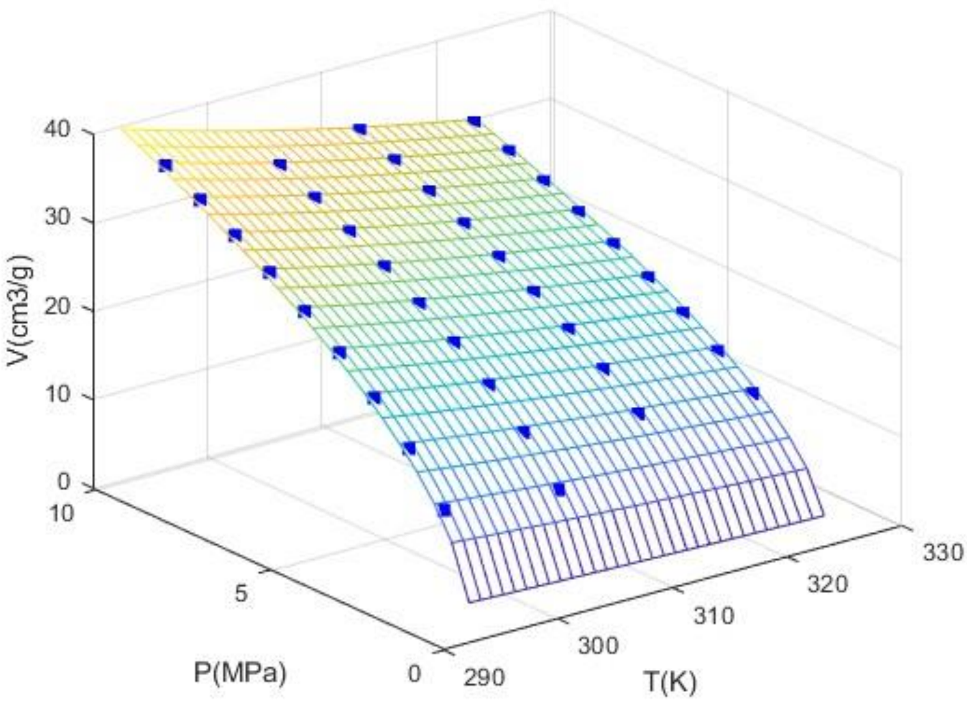

Figure 1: The temperature-pressure-adsorption relationship of lean coal

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III. RESULTS AND DISCUSION

A. Adsorption thermodynamics

If a given adsorption capacity was given and the four constants of TPAE (A, B, D, b) were known, then Equation 9 can be derived into:

$$lnP = \frac{1}{\beta} ln\left[\frac{V\sqrt{MT}-A}{BT^{1.5}exp\left(\frac{\Delta}{T}\right)}\right] \qquad (2)$$

As can be seen from Equation 10, given a temperature T and adsorption volume V, the pressure value P at this temperature T and this fixed adsorption volume V can be calculated.

B. Clausius-Clapeyron equation

The indefinite integral expression of the Clausius-Clapeyron equation of adsorption is

$$lnP = \frac{\Delta_g^l H_m}{R}\frac{1}{T} + C \qquad (3)$$

Where, $\Delta_g^l H_m$ is the enthalpy of molar change, which is equal in magnitude to the heat of molar adsorption, which is the isosteric adsorption enthalpy with one mole adsorption amount as the comparison base. The subscript "m" represents the mole. The subscript "g" indicates the initial state is gas; Superscript "l" indicates the final state is liquid. Based on Equation 3, the lnP vs 1/T should be a straight line, to the slop of this line describing the direction and degree of the enthalpy of molar adsorption.

C. Unit isosteric adsorption enthalpy

Equation 2 and the parameters in Table 2 are used to calculate the pressure P and temperature T while the adsorbed amount is set as 15 cm^3/g. And the calculated results are depictured in Figure 2 according to the Clausius-Clapeyron equation.

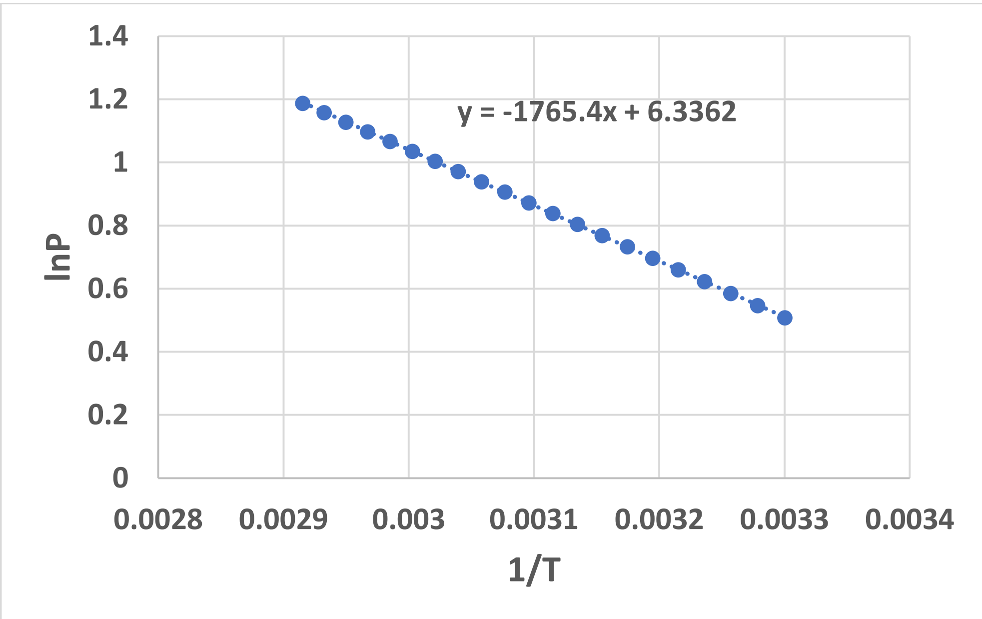

Figure 2: The lnP vs 1/T plotting of lean coal under 15 cm^3/g isosteric adsorption

Therefore, the unit isosteric adsorption enthalpy (UIAE) can be calculated as the following equation:

$$UIAE = \frac{-1765.4*0.008314}{15} = -0.9785 KJ.mol^{-1}.cm^{-3}.g \qquad (4)$$

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D. The direction of the adsorption enthalpy

The slops of lnP vs 1/T plot in Figure 2 are negative. Based on the indefinite integral expression of the Clausius-Clapeyron equation of adsorption, Equation 3, the most important inequality must be:

$$UIAE < 0 \quad (5)$$

Therefore, the adsorption process is an exothermic process.

E. The degree of the adsorption enthalpy

The UIAE is related to the adsorption capacity. Table 3 listed the different UIAE values at corresponding adsorption capacity.

TABLE 3: DIFFERENT UIAE AT DIFFERENT ADSORPTION CAPACITY

AA	UIAE	AA	UIAE
1	-14.678	11	-1.334
2	-7.339	13	-1.129
3	-4.893	15	-0.979
4	-3.669	17	-0.863
5	-2.936	19	-0.773
7	-2.097	21	-0.699
9	-1.631	25	-0.587

Where:
AA: Adsorption amount, cm^3/g
UIAE: Unit isosteric adsorption enthalpy, $KJ.mol^{-1}.cm^{-3}.g$
The data in Table 2 is depicted in Figure 3.

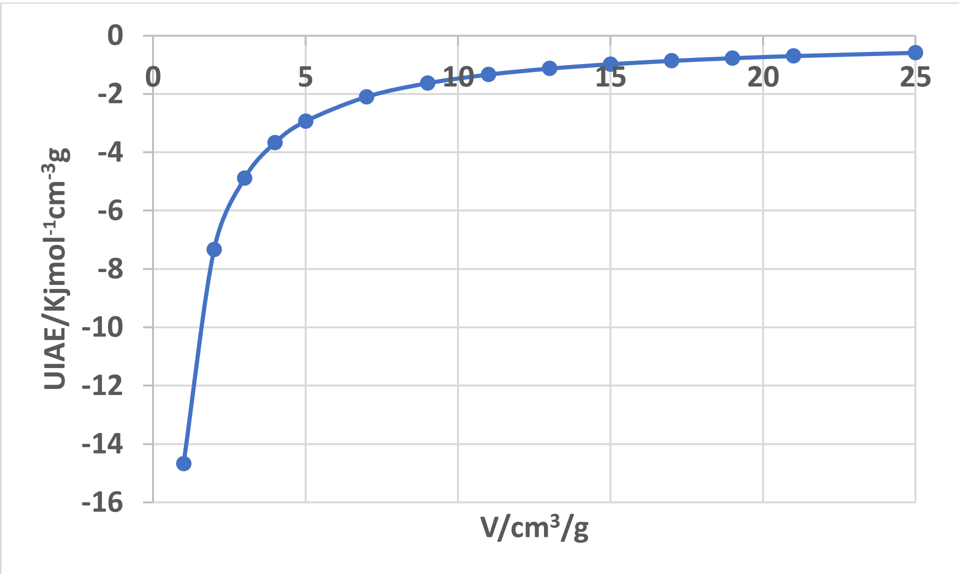

Figure 3: The relationship between the UIAE and adsorption capacity of lean coal

With the increase of adsorption capacity, the UIAE decreases. This phenomenon proves three things: the adsorbed surface is not smooth, there is an interaction force between the adsorbed molecules, and physical adsorption could be either monolayer or multilayer depending on which situation could release more energy.

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F. The reverse process of adsorption

The reverse process of adsorption is desorption. Adsorption is an exothermic process, so it can be carried out spontaneously. Desorption is an endothermic process, so it cannot be carried out spontaneously. Energy needs to be obtained from the environment to proceed. The data of Unit isosteric desorption enthalpy (UIDE/ $KJ.mol^{-1}.cm^{-3}.g$) is depicted in Figure 4.

Because the UIAE decreases with the increase of adsorption capacity, the UIDE decreases with the increase of adsorption capacity too. The UIAE decreasing means less heat would be released with the increase of adsorption capacity. The UIDE decreasing means less energy would be needed with the increase of desorption capacity.

Therefore, both characteristics of the equilibrium between adsorption and desorption the UIAE and UIDE changing along with the amount hold the secret about foreign energy accumulation and internal energy transformation, which are necessary for the occurring of coal and gas outburst.

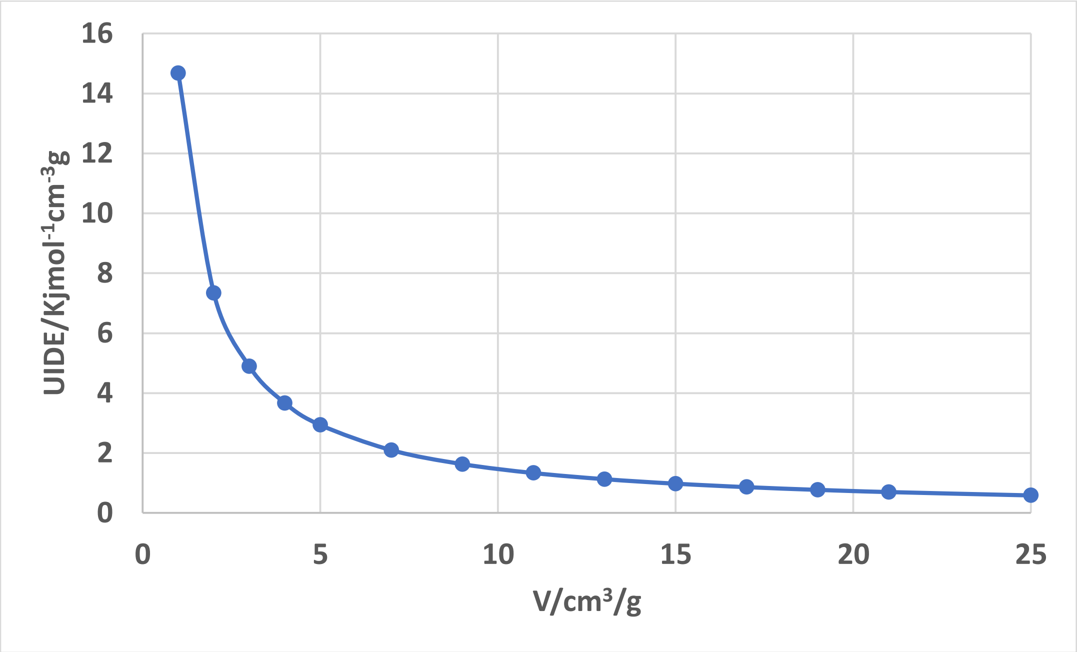

Figure 4: The relationship between the UIDE and desorption capacity of lean coal

IV. CONCLUSIONS

The isothermal adsorption data of a lean coal has been used to regress the parameters of a temperature-pressure-adsorption equation with acceptable accuracy.

The lnP vs 1/T plotting of lean coal under 15 cm^3/g isosteric adsorption indicates that the adsorption is an exothermic process, the desorption is an endothermic process.

Both the unit isosteric adsorption enthalpy (UIAE) and the unit isosteric desorption enthalpy (UIDE) have been calculated for different capacities.

Both UIAE and UIDE decrease with the increase of capacity. The UIAE decreasing means less heat would be released with the increase of adsorption capacity. The UIDE decreasing means less energy would be needed with the increase of desorption capacity.

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REFERENCES

[1] WANG Hao, JIANG Chenglin, YANG Feilong. Study on the characteristics of initial gas release expansion energy of imitation structural coal[J]. Journal of Mining & Safety Engineering, 2012, 29(2):277-282.
[2] Wang Enying. Prediction of gas geology in high-gas mine coal and gas outburst area[J]. Safety in Coal Mines, 2006, (10): 42-44.
[3] Wang Hongtu, Xian Xuefu, He Jianmin, et al. Discussion on the use of temperature index to predict the outburst hazard of the boring face[J]. Journal of Chongqing University (Natural Science Edition), 1999, 22(2): 34-38.
[4] ZHANG Jiayong, LUO Xinrong, GUO Liwen. Analysis of the causes of abnormal temperature change of coal body during gas outburst[J]. Coal Technology, 2011, 30(9): 88-90.
[5] Yang Tao, Nie Bai Sheng. Study on temperature change during gas adsorption by coal particles[J]. Journal of China Coal Society, 2015, 40(S2):380-385.
[6] ZHAO Wenfeng, XIONG Jianlong, ZHANG Jun, et al. Distribution law of tectonic coal and its influence on coal and gas outburst[J]. Coal Science and Technology, 2013, 41(2): 52-55.
[7] Jiang Jiayu, Lei Dongji, Xie Xiangxiang, et al. Study on pore structure and gas coupling characteristics of structural coal[J]. Journal of Safety and Environment, 2015, 15(1):123-128.
[8] CUI Yongjun, ZHANG Qingling, YANG Xilu. Adsorption performance and equal amount of heat adsorption of different coals[J]. Natural Gas Industry, 2003, 23(4): 130-131.
[9] Dong Li, Qinghua Ma, Xeumei Zhang, Yaling Wei, Jingyuan Hao. Study on the calculation and application of the unit isosteric adsorption enthalpy. International journal of innovative research in advanced engineering, 2022, Volume 9, issue 11, pages 453-458. //doi.org/10.26562/ijirae.2022.v0911.03
[10] Xeumei Zhang, Dong Li, Qinghua Ma, Zheng Wang, Jingyuan Hao. Study on a comparison of the Clausius-Clapeyron equations for desorption and adsorption. International journal of innovative research in advanced engineering, 2022, Volume 9, issue 12, pages 459-463. //doi.org/10.26562/ijirae.2022.v0912.01
[11] Qinghua Ma, Dong Li, Xuemei Zhang, Yaling Wei, Jingyuan Hao. Study on adsorption and desorption characteristics of normal coal and deformed coal with different stratification at the same location. International Advanced Research Journal in Science, Engineering and Technology, 2023, Volume 10, Issue 1, page 41-45. DOI: 10.17148/IARJSET.2023.10107

BIOGRAPHY

Wang Zhen, male, 1990-, graduated from Yinchuan College of China University of Mining and Technology, Yinchuan, Ningxia, China. Majoring in chemical engineering and technology, engaged in the research of efficient and clean utilization technology of coal.