



ORIGINAL RESEARCH ARTICLE

# Thermodynamic Analysis of Hydrogen Storage Process of Activated Carbon

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## ABSTRACT

The adverse effect of thermal effect in hydrogen storage process is one of the key problems that hydrogen adsorption storage needs to be applied to new energy vehicles. In this paper, the thermodynamic analysis model of activated carbon adsorption hydrogen storage process is introduced, including the adsorption isotherm model, the thermodynamic calculation of adsorption heat and the equation of gas state. The method of selecting the adsorption isotherm model and the selection method of the adsorption heat in the adsorption process, the applicability and selection of the gas state equation under different hydrogen storage conditions are discussed.

**KEYWORDS:** activated carbon; adsorption; hydrogen storage; thermodynamics

## 1. Introduction

### 1.1. Research background and significance

#### 1.1.1 Research background

Hydrogen, because of its many excellent characteristics and known as the 21st century green new energy. First, the hydrogen energy has a high calorific value, burning 1kg of hydrogen can produce  $1.25 \times 10^6$  kJ of calories, equivalent to 3kg of gasoline or 4.5kg of coke completely burn the heat generated. Second, the hydrogen after the release of the product is water, environmental friendly and pollution-free, green clean energy; In addition, hydrogen is the most abundant elements of the universe, a wide range of sources, through solar energy, wind energy, geothermal energy and other natural water can be produced for renewable energy, will not dry up. At present, many countries in the world are stepping up the deployment of hydrogen energy strategy to meet the arrival of the era of hydrogen economy, such as United States for the scale of hydrogen production FutureGen plan, Japan's NewSunshine and the European Framework program.

Lasting urban air pollution, demand for transportation of lower or zero emissions, reduced demand for foreign oil imports, carbon dioxide emissions and global climate change, storage of renewable energy supply demand and other factors of the convergence of increased hydrogen can be economically attractive [1].

At present, the use of hydrogen has made great progress. The successful development of liquid hydrogen engines has made the application of hydrogen into the aerospace field, and the many advantages of hydrogen can make the development of hydrogen fuel-driven railway locomotives and general automobiles very active. BMW hydrogen 7 series of hydrogen-powered vehicles have achieved mass production, but this technology is also difficult to popular, the main bottleneck is the storage and transportation of hydrogen. Hydrogen is very active, with the existing technology is difficult to keep it long and stable in the storage tank, if the hydrogen car does not open a month, inside the hydrogen will be exhausted [2]. In addition, hydrogen is still a flammable and explosive gas, in use must ensure safety, therefore, a safe, high energy density (including the volume of energy density and weight energy density), low cost, long life of hydrogen storage, the application of transportation technology has become increasingly urgent [3].

Traditional hydrogen storage methods are mainly gaseous and liquid two. Gaseous way is more simple and convenient, but also the current storage pressure is less than 70MPa hydrogen commonly used method, but the smaller bulk density is a serious technical defects in the method, and gaseous hydrogen in the transport and use of the process

there is also a great potential for security risks. The bulk density (70 kg / m<sup>3</sup>) of the liquid hydrogen storage method is high, but the liquefaction of the hydrogen gas needs to be cooled to a low temperature of 20K. This process consumes about 25% to 45% of the stored hydrogen energy. And the use of liquid hydrogen harsh conditions, the insulation requirements of high storage tanks, is currently limited to the application in the field of space technology. The use of hydrogen storage material and hydrogen reaction to generate solid solution and hydrogenation of solid hydrogen storage method, can effectively overcome the lack of two kinds of gas and liquid storage methods, and the storage volume of hydrogen storage density, high security, transportation convenience. According to the development trend of technology, the future of hydrogen storage research is focused on the new high-performance large-scale hydrogen storage materials, the current research is more extensive and in-depth porous adsorption of hydrogen storage materials [4].

Porous solid material hydrogen storage, because of its low working pressure, storage container, light weight, shape choice and other advantages, as the current hydrogen storage materials development and research hot spots. As the porous adsorbent for hydrogen storage, there are basically four kinds of porous materials such as carbon-based porous materials, non-carbon nanotube-based materials, mineral porous materials and metal organic materials.

In this paper, thermodynamics study was carried out on the thermal effect of hydrogen storage tank in hydrogen storage tank.

### 1.1.2 Research significance

The world's energy consumption is huge, and showing a significant growth trend. In recent years, people have come to realize the importance of energy structure for social development. There have been two major changes in the energy structure of human history: the first of which occurred in the late nineteenth century, where the fuel wood was replaced by coal; the second was replaced by oil in the 1970s as the main source of oil. Today, natural gas consumption is showing a straight line of growth [5]. From the replacement of the energy structure can be seen from the fuel wood, coal to the present oil, natural gas, which gradually reduce the carbon content, hydrogen content is getting higher and higher, their hydrocarbon atomic ratio were fuel wood: coal : oil: natural gas is about 0.1: 1: 2: 4. It can be seen that the trend of human energy development is to gradually replace the carbon, and ultimately into the era of carbon-free energy. For hydrogen, the hydrogen /carbon ratio tends to be infinite. From a long-term point of view, solar and nuclear fusion will be the ultimate energy of mankind, hydrogen isotope is its main raw material. Hydrogen itself is also responsible for the task as a vehicle energy carrier, so hydrogen can be said to be human eternal fuel, the development and utilization of hydrogen energy related to the sustainable development of human society, research significance is self-evident.

Compared with other energy sources, hydrogen has a high value of heat, pollution, a wide range of sources and many other excellent features [6]. The use of hydrogen can effectively alleviate the gradual loss of fossil fuels, greatly reducing greenhouse gas emissions.

Activated carbon hydrogen storage is in the low temperature (77-273K), high pressure (1-10Mpa) under the use of ultra-high specific surface area of activated carbon as adsorbent adsorption hydrogen storage technology. Compared with other hydrogen storage technology, super-activated carbon hydrogen storage is economical, high hydrogen storage capacity, desorption fast, long cycle life and easy to achieve large-scale production and other advantages, is a potential hydrogen storage method [7].

## 1.2. Thermodynamics of Adsorption Process

When the hydrogen storage system is inflated, temperature and pressure of the activated carbon bed have a great influence on the hydrogen storage capacity. Therefore, the thermodynamics of hydrogen storage process of the activated carbon is studied by a variety of experimental and theoretical methods.

NYSERDA and NYGAS co-sponsored by United Carbon Corporation and AGLARG International Cooperative Organization have been working on technical research of adsorption and storage of automotive fuels. One of its main efforts is to study the effects of heat absorption on gas storage and to reduce the thermal effects of adsorption [9].

Zhou Li, who use AX-21 activated carbon adsorption hydrogen storage study, proposed adsorption heat effect is usually refers to the same amount of adsorption heat. And the average adsorption heat of AX-21 activated carbon adsorbed storage was 6.4kJ /mol. The adsorption isotherm of hydrogen on the activated carbon in the range of 77K to 298K and 0-7MPa is first measured by the volumetric method. The results show that the Langmuir equation and the Virial equation are well explained in a certain temperature and pressure range as a result, the Dubinin-Astakhov equation best expresses the experimental data throughout the test range [8].

MalekLam et al. have shown that there is a significant temperature gradient in the axial and radial directions of the hydrogen storage tank during the adsorption process, and the highest temperature appears in the inflatable port. The slower inflation rate has no obvious advantage over the faster charge rate, while the higher inflation pressure is favorable for inflation. During the desorption process, the hydrogen storage tank has a temperature gradient in the axial direction

and the lowest temperature appears at the vent. The temperature difference between the vent and the bottom of the hydrogen storage tank is more than 30 ° C during rapid desorption [10].

### 1.3. Methodology

In this paper, the thermodynamic analysis model of activated carbon adsorption hydrogen storage process is introduced, including the adsorption isotherm model, the thermodynamic calculation of adsorption heat and the equation of gas state. The significance of the adsorption isotherm model and the selection method of the adsorption heat in the adsorption process, the applicability and selection of the gas state equation under different hydrogen storage conditions.

## 2. Thermodynamic model of adsorption hydrogen storage process

In order to study the thermodynamic changes in the process of hydrogen storage, it is necessary to use the mathematical model of adsorption isotherm model and gas state equation as the theoretical basis.

### 2.1. Adsorption isothermal model

#### 2.1.1 Necessity of adsorption isotherm study

IUPAC (International Pure Theory and Applied Chemistry Association) manual on the instructions: for the adsorption process, the first step is to determine the type of adsorption isotherms, and then determine the nature of the adsorption process [11]. Therefore, it is necessary to study the adsorption isotherm model which reflects the adsorption process.

The significance of the adsorption isothermal model is not only to find a convenient mathematical expression for the relationship between the amount of adsorption and the adsorption conditions, but also to understand the mechanism of microscopic adsorption [12]. On this basis, a certain theoretical model was used to process the experimental data to determine the maximum adsorption capacity, the adsorption heat effect, the specific surface area of the adsorbent and the pore volume, and other significant physical or thermodynamic quantities.

#### 2.1.2 Classification of adsorption isotherms

Adsorption isotherms are information sources about adsorbent pore structure, adsorption heat, and other physicochemical characteristics. The adsorption isotherms of the adsorbate can be obtained at a constant temperature and a wide range of relative pressure conditions. Correctly determine the type of adsorption isotherms, for the adsorption pore structure and other parameters of the calculation is very important. At present, many of the adsorption isotherms reported in the literature include a wide range of adsorbents and adsorbents. However, these adsorption isotherms still show a certain regularity. Classify according to the pressure and temperature of the adsorption line shape or adsorption.

##### (1) IUPAC adsorption isotherm type

IUPAC class 6 adsorption isotherms are shown in Figure 2-1.

Type I: indicates adsorption on micro-porous adsorbents;

Type II: indicates the adsorption on the macro-porous adsorbent, the interaction between the adsorbent and the adsorbate is strong;

Type III: indicates the adsorption on the macro-porous adsorbent, the interaction between the adsorbent and the adsorbate is weak;

Type IV: indicates the presence of capillary coagulation phenomenon of single layer adsorption;

Type V: that the presence of capillary condensation phenomenon of multi-layer adsorption;

Type VI: indicates a multi-layer adsorption on a non-porous adsorbent with uniform surface [13].

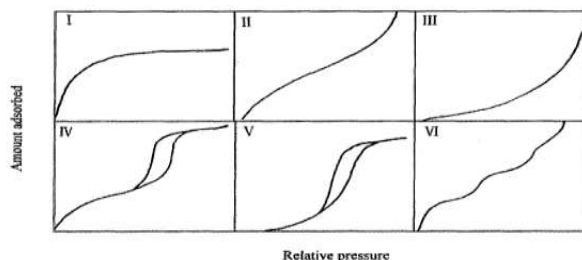


图 2-1 IUPAC 吸附等温线类型<sup>[47]</sup>

Figure 2-1 IUPAC adsorption isotherms classifications

## (2) Gibbs adsorption isotherms

The IUPAC classification curve shows that the amount of adsorption will always increase with the increase of pressure. However, with the deepening of the study of adsorption isotherm, some new types of gas-solid adsorption isotherms are not classified as IUPAC adsorption isotherm involving, in particular, the supercritical adsorption of gases.

Supercritical adsorption refers to the gas above the critical temperature occurs in the solid surface adsorption, above the critical temperature, the gas under normal pressure in the physical adsorption is relatively weak, so often to a very high pressure to have significant adsorption, so, The supercritical adsorption of gas, also known as high pressure adsorption.

In this new type of curve, there is a maximum value of adsorption. When the adsorption capacity reaches the maximum value, the adsorption capacity does not increase monotonically with the increase of pressure, so IUPAC has a limitation on the classification of gas-solid adsorption isotherms. In response to this finding, some scholars have proposed a new adsorption isotherm classification based on the Ono-kondo lattice theory model [14], which classifies Gibbs adsorption isotherms.

Gibbs adsorption isotherms are divided into five categories, as shown in Figure 2-2.

Class I represents adsorption isotherms on micro-porous adsorbents under subcritical or supercritical conditions. The adsorption isotherm under subcritical conditions is very similar to the classification of IUPAC, but the supercritical isotherm is the adsorption maximum.

Class II and III represent the adsorption isotherms when there is a strong and weak force between the adsorbent and the adsorbate on the macro-porous adsorbent, respectively. When the temperature is low, the adsorption isotherms have multiple adsorption steps. As the temperature increases, the adsorption isotherms become more gentle monotonically increasing curves, similar to the II and III of IUPAC. When the critical temperature is reached, the adsorption curve shows a very sharp maximum value. As the temperature continues to increase, the curve also has the maximum adsorption value, but the change trend is relatively gentle.

Class IV and V are the adsorption isotherms when there is strong and weak force between the adsorbent and the adsorbate in the meso-porous adsorbent, respectively. When the temperature is low, the adsorption isotherm appears stranded, but in the super critical temperature conditions do not necessarily occur.

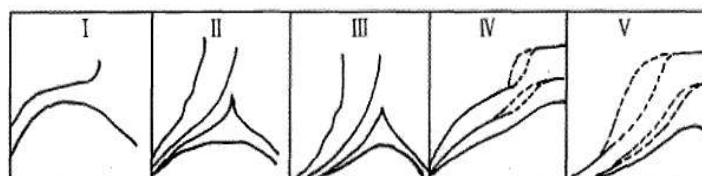
图 2-2 Gibbs 吸附等温线类型<sup>[47]</sup>

Figure 2-2 Categories of Gibbs adsorption isotherms

### 2.1.3 Comparison of adsorption isotherm model

At present, people still use the traditional adsorption theory such as Lanmuir equation, D-A or D-R equation, Virial equation to deal with supercritical adsorption of experimental data. The use of these models is based on the fact that the adsorption state of the gas above the critical temperature is similar to that of the saturated liquid below the critical temperature because the gas is not liquefied in a supercritical state.

The more common adsorption isotherm models include Herry's law, Lanmuir equation, virial equation, D-A equation, and so on.

## (1) Herry's Law

At the surface of the adsorbent, the coverage of the gas molecules is low, so that the Herry law can be used to express the adsorption phenomenon when it is considered that the adsorption phase is in the ideal state. The law thinks

$$n = K'P \quad (2-1)$$

Where  $n$  is the adsorption capacity (mmol/g),  $P$  is the equilibrium pressure (MPa), and  $K$  is the Herry law constant. Herry's law constant and temperature depend on the vantHoff equation:

$$d \ln K' / dT = \Delta H / RT^2 \quad (2-2)$$

(2) Lanmuir equation

The Lanmuir equation is the most common model used to describe the I-type isotherms, generally written in the following form:

$$\theta = n / n_0 = bP / (1 + bP) \quad (2-3)$$

Where n is the adsorption capacity; n<sub>0</sub> is the saturated adsorption capacity;  $\theta$  for the surface coverage. When the  $\theta$  tends to 0, the equation is transformed into Herry's law:

$$\lim_{P \rightarrow 0} (n / P) = bn_0 = K' \quad (2-4)$$

(3) Virial equation

Generally use the three-dimensional Virial equation to express a certain temperature range of hydrogen adsorption data:

$$\ln P = (c_0 + c_1n + c_2n^2) / T + \ln(n) \quad (2-5)$$

(4) D-A equation

$$n_a = n_{\max} \exp \left[ - \left( \frac{A}{E} \right)^b \right] \quad (2-6)$$

The results show that the Langmuir equation can be used as the isotherm at temperatures above 113K by comparing the adsorption temperature of the large temperature range of 77K-298K and 0-7MPa in the range of 77K-298K, model, but not for lower temperatures; the Virial equation is applicable to 153-298K, although it is not the best model for the whole set of data, but it can reliably determine the Herry constant, which can then be determined from the Vanthoff plot adsorption heat (average adsorption heat is 6510J / mol); and D-A equation in the entire experimental range can be a good expression of experimental data.

Therefore, the D-A (Dubinin-Astakhov) adsorption model is used to describe the adsorption isotherm of the activated carbon in the supercritical state (hydrogen supercritical temperature is 33.2K). Where the enthalpy factor a = 3080J / mol, the entropy factor b = 18.9j / mol / K. R = 8.314J / mol / K, T, P are the average temperature and pressure in the hydrogen storage tank, respectively. The limit adsorption capacity and ultimate pressure of hydrogen are n<sub>max</sub> = 71.6mol/kg, P<sub>0</sub> = 1470Mpa, D-A is the index b = very small pores corresponding to the majority of activated carbon, the index b to take 2. The absolute adsorption isotherms in different temperature and pressure ranges are shown in Figure 2-3. It can be seen from the figure, hydrogen in the activated carbon on the absolute adsorption capacity increases with the pressure increases, with the temperature rise.

It should be noted that the D-A equation is deviated from the experimental data under high pressure conditions, and the pore size distribution of the adsorbent has an effect on its surface properties. The D-A equation parameter b should be taken according to the different adsorbents. Therefore, we can consider the D-A equation for different operating pressure described in detail, and for different adsorbent microstructure to add, in order to achieve further amendments to the D-A equation, making it suitable for a wider range of pressure and temperature.

## 2.2. Thermodynamic calculation of adsorption heat

### 2.2.1 Mechanism of Adsorption Heat

During the process of hydrogen storage, the adsorption heat is directly influenced by the exothermic phenomenon when the hydrogen is adsorbed to the surface of the activated carbon. Therefore, it is necessary to study the adsorption heat.

Adsorption heat is one of the important physical quantities that characterize the physical and chemical properties of solid surfaces [15]. The size of the adsorption heat is directly related to the strength of the bond energy on the solid

surface. The stronger the surface bond is, the higher the adsorption heat is. The influence of external factors on the surface properties of solid can be studied by the change of adsorption heat.

The adsorption process is a spontaneous process in which the Gibbs free energy decreases during the adsorption process,  $\Delta G < 0$ . At the same time, the gas molecules are adsorbed, the original three-dimensional free movement to the solid surface, can only be two-dimensional movement, reduce the degree of freedom of movement. By the first law of thermodynamics:

$$\Delta G = \Delta H - T\Delta S \quad (2-7)$$

It can be seen that the adsorption process is  $\Delta H < 0$ , indicating that the adsorption process is an exothermic process.

The size of the heat of adsorption is the measure of the strength of adsorption. The adsorption heat of chemical adsorption is larger than that of physical adsorption. Therefore, the adsorption heat is also an important symbol to distinguish physical adsorption and chemical adsorption.

### 2.2.2 Calculation of adsorption heat

The same amount of adsorption heat can be calculated by the gas isothermal adsorption curve at different temperatures, and its size decreases with the increase of adsorption capacity. From the thermodynamic point of view, when the adsorption reaches equilibrium, the Gibbs free energy of the adsorbed mass and the adsorbed phase is equal.

$$G_g = G_a \quad (2-8)$$

When the amount of adsorption is constant, if the temperature changes slightly, the pressure at the time of adsorption equilibrium also changes accordingly. So when the new balance is reached, the formula as below:

$$dG_g = dG_a \quad (2-9)$$

Which is

$$-S_g dT + V_g dP = -S_a dT + V_a dP \quad (2-10)$$

From the above relation, if the isothermal equation is in the form of  $N = N(P, T)$ , when the pressure is  $P$  and the temperature is  $T$ ,

$$\left(\frac{\partial P}{\partial T}\right)_a = \frac{S_g - S_a}{V_g - V_a} = \frac{q_{st}}{T(V_g - V_a)} \quad (2-11)$$

The equivalent adsorption heat  $q_{st}$  on the surface area  $A$  of the solid adsorbent can be expressed as

$$q_{st} = T(V_g - V_a) \left(\frac{dP}{dT}\right)_{N,A} \quad (2-12)$$

Where  $N$  is the amount of adsorption on the surface area  $A$ . Assuming that the hydrogen is the ideal gas during the adsorption process,  $V_g \gg V_a$ , according to the ideal gas equation of state, equation (2-12) can be collated into:

$$q_{st} = \Delta H = -R \left[ \frac{d \ln P}{d(1/T)} \right]_N \quad (2-13)$$

According to the adsorption isotherm data, make  $\ln p$  on the  $1/T$  of the straight line, from its slope directly calculated  $q_{st}$  value. The D-A equation can describe the adsorption isotherm in a certain temperature and pressure range. Therefore, the equivalent adsorption heat of hydrogen adsorption on the activated carbon can be calculated by using the D-A equation.

According to the adsorption isotherm data of hydrogen in activated carbon in Fig. 2-3, a corresponding linear relationship between  $\ln p$  and  $1/T$  is obtained. The corresponding manifestations are shown in Fig. 2-4.

Absolute adsorption capacity of the same amount of adsorption heat can be calculated according to the linear slope of the calculation, the specific relationship between Table 2-1.

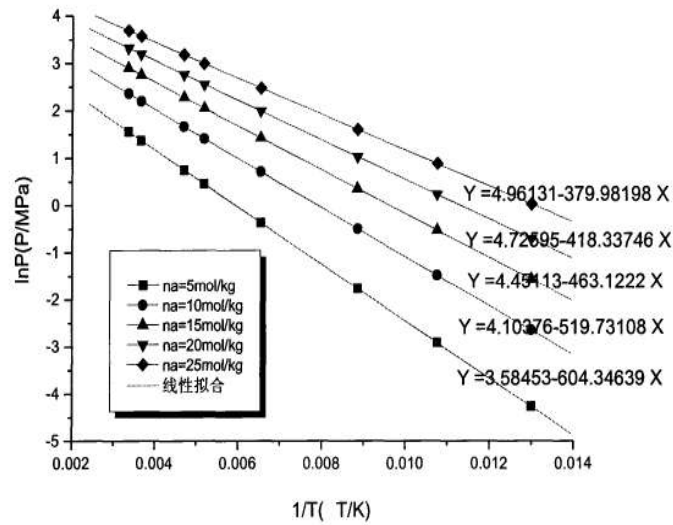


Figure 2-4 Adsorption heat of hydrogen adsorption on activated carbon

From the data in Table 2-1, it can be seen that the magnitude of the equivalent adsorption heat varies between 3159.39437Jmol<sup>-1</sup> and 5024.89245Jmol<sup>-1</sup> depending on the amount of absolute adsorption within a certain range, calculated from the set of data. The average adsorption heat under different absolute adsorption capacity is

$$q_{st} = \frac{\sum_{i=1}^5 -R \left[ \frac{d \ln P}{d(1/T)} \right]_{N_i}}{5} = -8.31459 \times (-477.1) = 3966.9 \text{ J/mol} \quad (2-14)$$

### 2.3. Gas state equation

For a certain amount of gas in equilibrium, its state is determined by the pressure  $p$ , the temperature  $T$  and the volume occupied by it, and the equation that expresses the relationship between these quantities is called the gas state equation. Different gases have different state equations. In general, the state equation of the actual gas is usually more complex and the equation of state of the ideal gas is very simple.

Although the complete ideal gas does not exist in practical applications, there are many actual gases, especially those that are not easy to liquefied and condensate gas (such as hydrogen, oxygen, nitrogen, and helium), because the helium molecules are not only small, and the interaction between the molecules is also small, but also the most difficult to liquefied all the gas, so it is the most gas in all the ideal gas.

#### 2.3.1 Ideal gas state equation

The ideal gas model refers to:

- (1) The molecules of the gas itself do not occupy the volume;
- (2) There is no interaction between molecules.

In reality, there is no ideal gas, but when the actual gas pressure  $p$  is small, the volume  $V$  is large, the temperature  $T$  is not too low, that is, away from the liquid state of thin, can be regarded as the ideal gas. The ideal gas equation, also known as the Clapeyron equation, is of the four forms of Clara Veron equation:

$$1 \text{ kmol: } pV_m = RT$$

$$n \text{ kmol: } pV = nRT$$

$$1 \text{ kg: } pv = R_g T$$

$$m \text{ kg: } pV = mR_g T$$

Where  $v$  is the specific volume and  $V_m$  is the molar volume ( $\text{m}^3 / \text{mol}$ ). Avogadro hypothesis: the same pressure and temperature of the ideal gas  $V_m$ , the same, under the standard,  $P_0 = 101.325\text{KPa}$ ,  $T_0 = 273.15\text{K}$ ,  $V_{m0} = 22.414\text{m}^3 / \text{kmol}$ ,  $V_m$  commonly used to represent the number.

The general form of the ideal gas equation of state is

$$p = \frac{R_g T}{v} \quad (2-15)$$

Where  $R_g$  is the individual gas constant and its relationship to the universal gas constant  $R$  is

$$R_g = \frac{R}{M} \quad (2-16)$$

$R_g$  is related to the gas species, and  $R$  is independent of the gas species.

The nature of the ideal gas can be summarized as follows:

- (1) The ideal gas follows the Kraiberian state equation;
- (2) Specific heat capacity and specific volume of heat capacity are only a function of temperature, and their differences are equal to (individual) gas constants.
- (3) Ideal gas thermodynamics and baking is only a function of temperature.

According to the ideal gas properties of the calculation of the thermodynamic properties of gas workers, the relationship between the various parameters of the most simple form, as long as the specific heat capacity of the material can be thermodynamic energy, enthalpy, entropy and other parameters of the calculation, easy to use.

### 2.3.2 Actual gas state equation

In the actual case calculation, there is a deviation when the ideal gas state equation is applied to the actual gas, since the basic assumption about the ideal gas is not true in the actual gas. Such as the experimental determination of 1 mol acetylene at 293K, 0.1MPa when the volume of 24.1 L, while the same at 293K, 1 mol acetylene in the pressure of 0.842MPa volume of 0.114 L, the volume difference is very large, it is not ideal gas.

To study the actual gas properties, we first come to the exact state equation.

There are two ways to study the actual gas state equation:

- (L) Directly using the experimental results obtained from a variety of thermodynamic data, according to the thermodynamic relationship between the state equations;
- (2) From the theoretical analysis, considering the behavior of gas molecules and the introduction of some parameters of the ideal gas state equation to be modified, the equation of the form, and the introduction of constant values are based on experimental data to determine. Often people refer to the actual gas state equation for the van der Waals equation and the Ridlik - Kwong equation.

- (1) van der Waals (van de räalsals) equation

In 1873, van der Vaars made the first meaningful natural gas equation) van der Waals equation. The van der Waals equation can give the relationship between the actual gas states change under high pressure and strong, and can be applied to the liquid state after the generalization. It is the simplest and most convenient one of many approximation equations. The van der Waals state equation takes into account the molecular self-occupied volume and the intermolecular interaction force, and corrects the ideal gas state equation: the molecular self-occupied volume reduces the free space of the molecule, and the frequency of the molecular collision vessel wall at the same temperature Increased, and thus the corresponding increase in pressure; the mutual attraction between molecules to the molecular collision vessel wall strength weakened, the pressure decreases. After considering the two effects, the gas pressure is:

$$p = \frac{RT}{v-b} - \frac{a}{v^2} \quad (2-17)$$

The constants  $a$  and  $b$  introduced on the basis of the ideal gas equation of state are called van der Waals constants

The value can be determined by the experimental data.

- (2) Ridley grams of a Kuang equation (R-K equation)



Proposed in 1949 and improved on the van der waals equation, closer to the actual situation:

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)} \quad (2-18)$$

Among them

$$a = 0.42748 \frac{R^2 T_c^2}{P_c} T_r^{-0.5}, \quad b = 0.08664 \frac{RT_c}{P_c} \circ T_r = T/T_c$$

Into the hydrogen critical temperature and critical pressure values, obtained

$$a = 6090 T_r^{-0.5}, \quad b = 9.018 \times 10^{-3}$$

The difference between the actual gas and the ideal gas is commonly used as a compression factor Z:

$$Z = \frac{Pv}{R_g T} = \frac{PV_m}{RT}$$

For the van der Waals equation, the squeezing factor Z satisfies:

$$Z^3 - (1+B)Z^2 + AZ - AB = 0$$

For the R-K equation, the compression factor Z is satisfied:

$$Z^3 - Z^2 + (A - B - B^2)Z - AB = 0$$

Among them

$$A = a \frac{P}{R_g^2 T^2}, \quad B = b \frac{P}{R_g T}$$

### 3. Conclusions

In this paper, the thermodynamics model of adsorption isotherm model and gas state equation is studied, which is the basis for the simulation and thermodynamics of hydrogen storage process.

(1) First, the necessity and significance of studying the adsorption isotherm are introduced, and the adsorption isotherm type is described for different classification methods. By comparing the common adsorption isotherm model including Herry's law, Lanmuir equation, Virial equation and D-A equation, this paper will use D-A (Dubinin-Astakhov) adsorption model which can express the experimental data well to describe the activated carbon in supercritical state adsorption isotherms.

(2) When the hydrogen is adsorbed to the surface of the activated carbon, the heat generated by the heat is directly affected by the heat of adsorption. In a certain range, the size of the same amount of adsorption heat varies depending on the amount of absolute adsorption. According to the adsorption isotherm data, make 1 np on the 1/T of the straight line, from its slope directly calculated the value of the same amount of adsorption heat. The average adsorption heat under different adsorption capacity is 3966.9J / mol calculated from the D-A adsorption isotherm data.

(3) To study the gas properties of the first to get accurate state equation. The state equation of the actual gas is usually more complex, and the van der waals equation and the RK equation which are often cited are introduced in this paper, and the equation of the ideal gas state is usually described, the corresponding compression factor.

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