

# A New Method to Calculate the Absolute Amount of High-Pressure Adsorption of Supercritical Fluid

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**ABSTRACT:** In the paper we developed a new method to determine the absolute amount of adsorption. This method relies on the excess adsorption isotherm and the density profile in the pore of one material. To compute the density profile and decrease complex calculation of obtaining the absolute amount of adsorption we introduced Simplified Local-Density (SLD) model. A few of appropriate parameters were acquired to calculate the density profile through SLD models the adsorption isotherm of methane on AX-21 activated carbon. In these parameters specific surface area and slit width is close to the true value of the AX-21 activated carbon. And we found SLD can accurately simulate the adsorption of supercritical methane on activated carbon and the precision rises up as temperature raises. The corresponding application of our method on adsorption of methane on AX-21 activated carbon was introduced at different temperature from 233 to 333K. The absolute isotherms of adsorption calculated by our method are reasonable when compared to other results.

**KEY WORDS:** Adsorption, Activated carbon, Supercritical fluid.

## INTRODUCTION

The research of adsorption of SuperCritical Fluid (SCF) has attracted the interest of investigators for a long time, because the adsorption of SCF has some vital important applications such as natural gas storage, hydrogen storage, the separation and purification of lower hydrocarbons and Supercritical Fluid Extraction (SFE). Many researchers have studied the adsorption of SCF with various theoretical methods and experiment. *Rangarajan et al.* developed Simplified Local Density (SLD) theory to model the adsorption over large pressure ranges, which has no computationally intensive [1]. *Aranovich & Donohue* calculated the adsorption isotherms of SCF with Ono-Kondo theory and the model reflects a maximum

adsorption with increasing pressure [2, 3]. They also found the adsorption of SCF has a two-layer character. *Murata & Kaneko* determined the absolute amount of high-pressure adsorption of supercritical methane by iteration procedures using the mean density of the adsorbed phase and Langmuir equation [4]. *Zhou et al.* confirmed the reversibility of physical adsorption for supercritical methane on active carbon and developed a method can describe the absolute adsorption with Dubinin-Astakhov equation and the limiting condition of supercritical adsorption [5-8]. *Kaneko & Murata* researched the micro pore filling of supercritical gas with replacing saturated vapor pressure with quasi-saturated vapor

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pressure for Dubinin-Radushkevich equation [9]. *Tan & Gubbins* investigated the adsorption behavior of gases at temperatures above the critical value with NonLocal Density Functional Theory (NLDFT) and Grand Canonical Monte-Carlo (GCMC) simulation and studied the influence of temperature and pore size on excess adsorption isotherms [10]. *Heuchel et al.* predicted the adsorption of pure-component and binary mixtures of methane and carbon dioxide on active carbon with GCMC and it was possible to predict in good agreement with experiment [11]. *Talu & Myers* modeled the adsorption of supercritical gas with molecular simulation and they argued absolute simulation variables must be converted to excess variables in order to compare simulations with experimental data [12]. Although the abundant research for SCF is existed in many fields, we do not list all here anymore for saving space.

Generally over the past decades, we already has some methods to research the adsorption of SCF on many materials, but the mechanism of supercritical gas adsorption is not completely established for lacking of abundant and accurate experiment data and a perfect theory. Therefore the state and structure of an adsorbed phase are not sufficiently understood and the density and volume of the adsorbed phase is unknown exactly. Naturally the absolute adsorption amount cannot be calculated with the most right theory. But among the past studies some researchers tried their best to investigate the relation between the absolute adsorption and excess adsorption. *Murata & Kaneko* calculated the absolute adsorption amount of supercritical methane with using the mean density of the adsorbed phase which is determined by excess adsorption isotherm [4]. And this method completely removed the maximum of excess isotherms. But during the calculation they assumed the absolute adsorption isotherm is Langmuir type to acquire two important parameters, and we don't know if Langmuir equation can describe the absolute adsorption of SCF, especially high-pressure adsorption of SCF, so this method has an obvious defect. They also acquired the absolute adsorption amount in previously their research with assuming the adsorbed phase is liquid like and has the liquid density [4], but the method cannot provide the monotonous adsorption isotherms for liquid density is much bigger than the true density of adsorbed phase. *Nikolaev et al.* and *Reich et al.*

tried to improve the method of regarding adsorbed phase density as liquid density; they assumed that the adsorbed phase consists of molecules having the Van der Waals exclusion value  $b$ , but they failed [13, 14]. *Salem et al.* and *Neimark et al.* calculated the absolute adsorption amount with presuming the volume of the adsorbed phase is equal to the pore volume, and they got a monotone adsorption isotherm for porous materials, but the method can't be applied to non-porous materials and treat the pore volume as the volume of adsorbed phase for none definite reason [15, 16]. *Myers & Monson* tried to achieve the link of absolute adsorption and excess adsorption with acquiring the accurate void volume of experimental system, but this volume cannot be acquired precisely by experiment [17]. *Do & Do* proposed a method to use the integration of a pore volume distribution to calculate the adsorbed phase volume, and they treated the radius of the pore below which the adsorption density is different from the bulk density everywhere as the limit of integration [18]. Actually we don't know how to get the right value of the radius for different temperature and pressure, so this method comes across a technological problem.

So far there is no a proper way to calculate the absolute adsorption of SCF. Though the absolute adsorption can be acquired by experiment, it is an extremely complicated work and has no a wide range of applications [19]. Hence we need a better approach to obtain the absolute amount of adsorption for avoiding those problems. In this paper, we describe a method to calculate the absolute amount of SCF adsorption, and the application on activated carbon which has high specific surface area will be shown over large temperature and pressure ranges.

## THEORITICAL SECTION

### *The method to calculate the absolute amount of adsorption* *Excess adsorbed amount and Absolute adsorbed amount*

According to the definition of excess adsorption and absolute adsorption, excess adsorbed amount and absolute adsorbed amount has an expression, as follows:

$$n_{\text{ex}} = \int_{V_{\text{ads}}} (\rho(r) - \rho_{\text{bulk}}) dr \quad (1)$$

$$n_{\text{abs}} = \int_{V_{\text{ads}}} \rho(r) dr \quad (2)$$

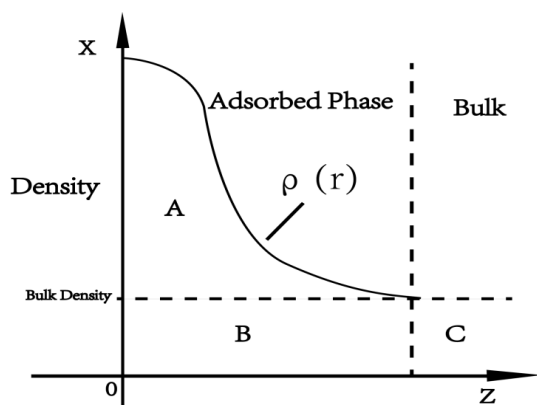


Fig. 1: The relation of excess adsorption and absolute adsorption.

Where  $V_{\text{ads}}$  is the volume of adsorbed phase,  $\rho(r)$  is the density profile of adsorbed phase,  $\rho_{\text{bulk}}$  is the density of bulk fluid. Obviously  $\rho_{\text{bulk}}$  is constant, so we can get the relationship:

$$n_{\text{abs}} = n_{\text{ex}} + \rho_{\text{bulk}} V_{\text{ads}} \quad (3)$$

Fig. 1 shows the relation between excess adsorption and absolute adsorption. Part A represents excess adsorption, part A and B expresses absolute adsorption.

### Method

Apparently we can calculate the absolute adsorbed amount under the precondition of having excess adsorbed amount and the volume of adsorbed phase through Eq. (3). And the excess amount of adsorption can be obtained by the adsorption experiment, the core to acquire the absolute mass is to determine the value of  $V_{\text{ads}}$ .

We assume the volume of adsorbed phase for unit mass has such an expression:

$$V_{\text{ads}} = S_A \cdot H \quad (4)$$

Where  $S_A$  is the specific surface area of one material,  $H$  is the thickness of adsorbed phase. According to Fig. 1 the value of  $H$  locates at the interface between adsorbed phase and bulk phase. Hence we can obtain the value of  $H$  through solving the equation:

$$\rho(r)|_{r=H} = \rho_{\text{bulk}} \quad (5)$$

Actually there are two cases in pore of adsorbent for different temperature and pressure. One is that the density of fluid is bigger than bulk density somewhere and is

less than bulk density at another place in the pore under the same temperature and pressure, and Eq. (5) has solution as well. The other is that the density of fluid is bigger than bulk density everywhere in the pore at the same temperature and pressure, which means Eq. (5) has no solution. Figs. 2 and 3 present the situation. For the first situation the value of  $H$  is the solution of Eq. (5), and we need choose an appropriate one if the solution is not unique. The details will be discussed later. For the second situation the thickness of adsorbed phase obviously is half of the pore diameter.

Now we discuss how to distinguish the situation belongs to which case in the pore for each temperature and pressure. Our method to differentiate the situation has three steps. The first step is getting the density profile under several temperatures and pressure by theoretical calculation and the minimum of each density profile and then finding the relation between the minimum density and pressure through data fitting. In second step we get the link of bulk density and pressure by data fitting. The third step is to achieve the intersection of two curves which have been obtained by the corresponding equations acquired by step 1 and step 2. At this moment two cases may exist (Figs. 4 and 5). For the first one (Fig. 4) the Eq. (5) has no solution when the pressure below the pressure of intersection. So the value of  $H$  is half of the pore diameter for the pressure to below the pressure of intersection and can be determined by solving Eq. (5) for the pressure to above the pressure of intersection. It is on the contrary for the second case (Fig. 5). Once the intersection has been determined we can get the different value of  $H$  for different pressure under the same temperature. And the specific surface area can be obtained precisely with the current technology. Thus we can calculate the volume of adsorbed phase through Eq. (4). And then we can determine the absolute amount of adsorption.

Obviously to calculate the absolute amount of adsorption it is important to achieve the density profile for adsorbed phase. So far it is not possible to get the density distribution under the current experiment technology. However some theories can calculate the density profile reasonably, such as molecular simulation, Density Functional Theory (DFT), NLDFT and SLD theory. Molecular simulation, DFT and NLDFT can more accurately imitate the adsorption character of material

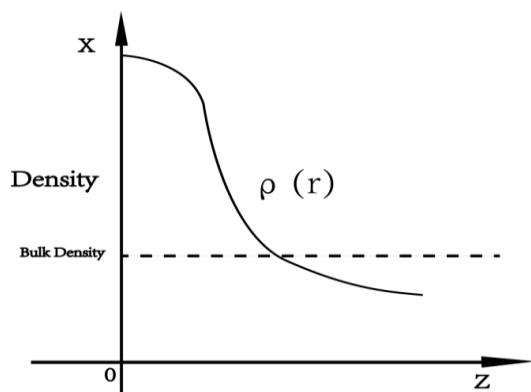


Fig. 2: The value of density profile and the value of bulk density have intersection.

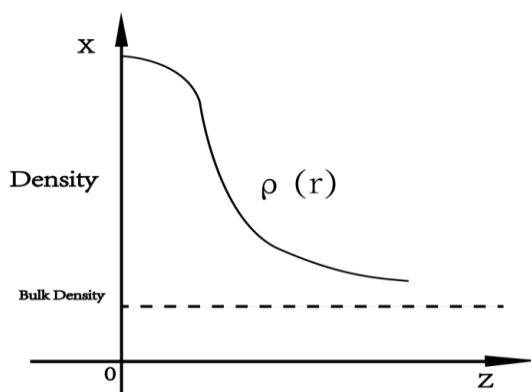


Fig. 3: The value of density profile and the value of bulk density have no intersection.

and obtain the density profile than SLD, but they are computational complexity and time consuming [20]. It was proved that SLD model can reflect the character of high-pressure adsorption for SCF with higher precision, which has no computationally intensive and the time consuming is much less than the other methods and the SLD model can serve as an engineering method to model the adsorption of SCF and acquire the density distribution [20-23]. Therefore we choose SLD theory to accomplish our work. SLD model and the method to calculate the density distribution for one material will be shown in the next section.

### SLD model

SLD model assumed the adsorbent consists of a rectangular shape slit pore and the adsorbate molecular resides in the slit pore (Fig. 6). The distance between

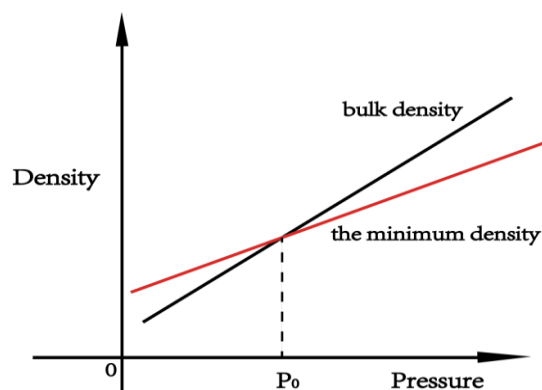


Fig. 4: The intersection between bulk density and the minimum density (case one).

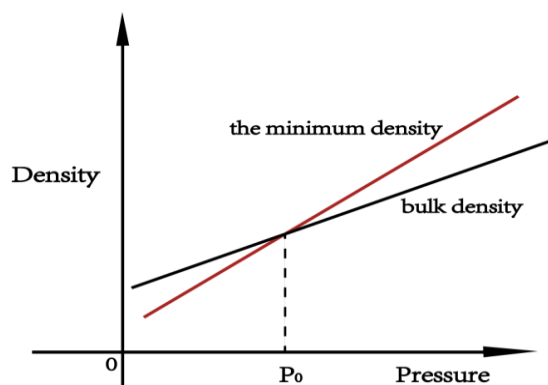


Fig. 5: The intersection between bulk density and the minimum density (case two).

the two slit surfaces is  $L$ , and a molecule's position is  $Z$  in the slit pore and the position is perpendicular to surface of slit pore.

When interaction between adsorbent molecular and adsorbate molecular reaches the equilibrium state, the chemical potential of  $Z$ -position is composed of fluid-fluid and fluid-slit pore surface and equal to bulk fluid's chemical potential[1]:

$$\mu(z) = \mu_{ff}(z) + \mu_{fs}(z) = \mu_{bulk} \quad (6)$$

The chemical potential can be calculated by fugacity:

$$\mu_{bulk} = \mu_0(T) + RT \ln \left( \frac{f_{bulk}}{f_0} \right) \quad (7)$$

$$\mu_{ff}(z) = \mu_0(T) + RT \ln \left( \frac{f_{ff}(z)}{f_0} \right) \quad (8)$$

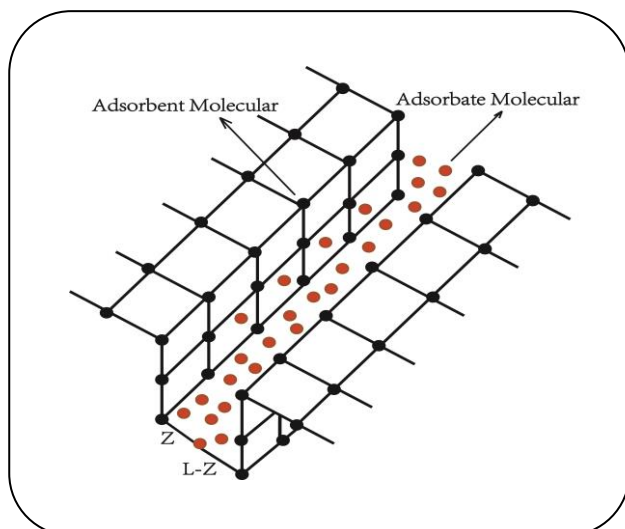


Fig.6: The pore model of SLD.

The chemical of interaction between fluid molecular and adsorbent molecular are given as:

$$\mu_{fs}(z) = N_a \left[ \psi^{fs}(z) + \psi^{fs}(L-z) \right] \quad (9)$$

Where  $N_a$  is Avogadro's number,  $\psi$  is potential. The potential of fluid-solid interaction,  $\psi^{fs}(z)$  can be calculated by follow equation[22,24]:

$$\psi^{fs}(z) = 4\pi n \epsilon_{fs} \sigma_{fs}^2 \left( \frac{\sigma_{fs}^{10}}{5(z + \sigma_{ss}/2)^{10}} - \frac{1}{2} \sum_{i=1}^4 \frac{\sigma_{fs}^4}{(z + \sigma_{ss}/2 + (i-1) \cdot \sigma_{ss})^4} \right) \quad (10)$$

Where  $\sigma_{ss}$  is the adsorbent interplanar distance,  $\sigma_{fs}$  is the distance interaction of adsorbate molecular and adsorbent molecular, generally  $\sigma_{fs} = (\sigma_{ff} + \sigma_{ss})/2$ ,  $\sigma_{ff}$  is the molecular diameter of gas,  $\epsilon_{fs}$  is the fluid-solid interaction energy parameter. Substituting Eqs. (7), (8) and (9) into Eq. (6) acquires the equilibrium equation of adsorption:

$$f_{ff}(z) = f_{bulk} \cdot \exp\left(-\frac{\psi^{fs}(z) + \psi^{fs}(L-z)}{kT}\right) \quad (11)$$

Where  $k$  is Boltzmann constant;  $k=1.3806505 \times 10^{-23}$  J/K. The Peng-Robinson Equation Of State (EOS) is more appropriate to reflect the repulsive force of fluid molecular [25], so we calculated the fugacity of adsorbate with Peng-Robinson EOS.

$$\frac{P}{\rho_{bulk} RT} = \frac{1}{(1 - \rho_{bulk} b)} \quad (12)$$

$$\frac{a(T) \rho_{bulk}}{RT \left[ 1 + (1 - \sqrt{2}) \rho_{bulk} b \right] \left[ 1 + (1 + \sqrt{2}) \rho_{bulk} b \right]}$$

$$\ln \frac{f_{bulk}}{p} = \frac{b \rho_{bulk}}{1 - b \rho_{bulk}} - \frac{a(T) \rho_{bulk}}{RT (1 + 2b \rho_{bulk} - b^2 \rho_{bulk}^2)} \quad (13)$$

$$\ln \left[ \frac{p}{RT \rho_{bulk}} - \frac{pb}{RT} \right] - \frac{a(T)}{2\sqrt{2}bRT} \ln \left[ \frac{1 + (1 + \sqrt{2}) \rho_{bulk} b}{1 + (1 - \sqrt{2}) \rho_{bulk} b} \right]$$

$$a(T) = \frac{0.457535 \alpha(T) R^2 T_c^2}{P_c} \quad (14)$$

$$b = \frac{0.077796 R T_c}{P_c} \quad (15)$$

Here we choose Gaseem's method to calculate  $\alpha(T)$  [26]:

$$\alpha(T) = \exp\left( (A + B T_r) \left( 1 - T_r^{C + D \omega + E \omega^2} \right) \right) \quad (16)$$

A, B, C, D and E are related parameters, their value is 2.0, 0.8145, 0.134, 0.508, and -0.0467. The value of acentric factor  $\omega$  is 0.0113 for methane [25]. The fugacity of adsorbed gas phase can be calculated by the equation[24-29]:

$$\ln \frac{f_{ff}(z)}{p} = \frac{b \rho(z)}{1 - b \rho(z)} - \frac{a_{ads}(z) \rho(z)}{RT (1 + 2b \rho(z) - b^2 \rho^2(z))} \quad (17)$$

$$\ln \left[ \frac{p}{RT \rho(z)} - \frac{pb}{RT} \right] - \frac{a(z)}{2\sqrt{2}bRT} \ln \left[ \frac{1 + (1 + \sqrt{2}) \rho(z) b}{1 + (1 - \sqrt{2}) \rho(z) b} \right]$$

The covolume  $b$  need to be adjusted for describing the repulsive interaction of adsorbed fluid under high pressure. Then Eq. (17) becomes:

$$\ln \frac{f_{ff}(z)}{p} = \frac{b_{ads} \rho(z)}{1 - b_{ads} \rho(z)} \quad (18)$$

$$\frac{a_{ads}(z) \rho(z)}{RT (1 + 2b_{ads} \rho(z) - b_{ads}^2 \rho^2(z))} - \ln \left[ \frac{p}{RT \rho(z)} - \frac{pb_{ads}}{RT} \right] -$$

$$\frac{a_{ads}(z)}{2\sqrt{2}b_{ads}RT} \ln \left[ \frac{1 + (1 + \sqrt{2}) \rho(z) b_{ads}}{1 + (1 - \sqrt{2}) \rho(z) b_{ads}} \right]$$

Table 1: The parameters of SLD-PR model represented the adsorption of methane on activated carbon.

Temperature (K)	Slit width (nm)	Specific surface area (m <sup>2</sup> /g)	$\epsilon_{fs}/k$ (K)	$\sigma_{ss}$ (nm)	$\sigma_{ff}$ (nm)	N (nm <sup>-2</sup> )
333	1.8	2820	59	0.335	0.38	38.2
313	1.8	2820	60.5	0.335	0.38	38.2
293	1.8	2820	63	0.335	0.38	38.2
273	1.8	2820	66	0.335	0.38	38.2
253	1.8	2820	69.5	0.335	0.38	38.2
233	1.8	2820	74	0.335	0.38	38.2

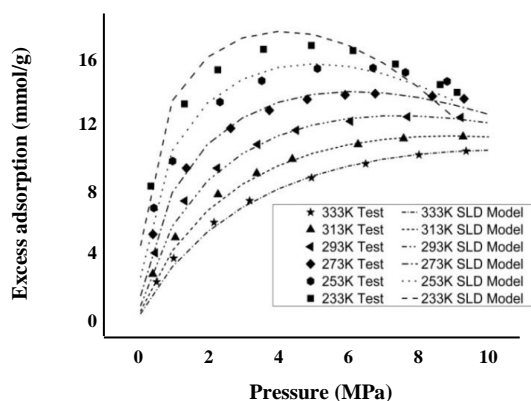


Fig. 7: SLD model representation for methane adsorption on AX-21 activated carbon.

$$b_{ads} = b(1 + A_b) \quad (19)$$

We used the expression introduced by *Chen et al.* to obtain  $\alpha_{ads}(z)$  [22]. By combining equations from (6) to (19), we can compute the density profile  $\rho(z)$ . According to definition of excess adsorption the adsorption capacity of the material can be calculated as follows:

$$n_{ex} = \frac{A}{2} \int (\rho(z) - \rho_{bulk}) dz \quad (20)$$

Where A is specific surface area. Generally there are six variables in this SLD model, they are slit pore width L, specific surface area A, the fluid-solid interaction energy parameter  $\epsilon_{fs}$ , the adsorbent inter planar distance  $\sigma_{ss}$ , the molecular diameter of fluid  $\sigma_{ff}$  and the number of adsorbent plane atoms per unit area n. Hence we can achieve the density profile at specific temperature and pressure if we obtain the value of those parameters for one material.

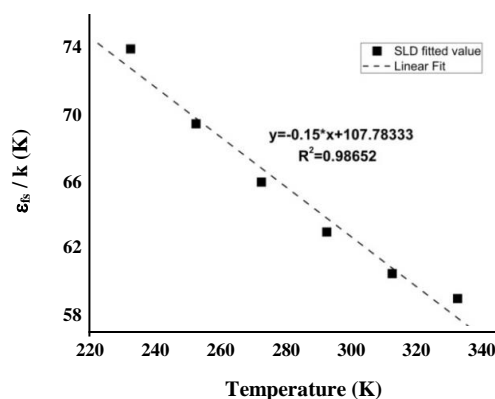


Fig. 8: The relation of SLD energy parameter and temperature.

### Application on the adsorption methane on AX-21 activated carbon

#### SLD Parameters for AX-21 Activated Carbon

The data of adsorption of methane on AX-21 activated carbon comes from *Zhou et al.* [7]. According to *Zhou et al.* the specific surface area of the activated carbon is about 3000 m<sup>2</sup>/g and its micro pore volume is about 1.5 mL/g [7]. We model the sorption isotherm comes from *Zhou et al.* [7] (Fig. 7) and obtain relevant SLD parameters (Table 1). On the whole SLD model can represent the adsorption of methane on the AX-21 activated carbon precisely. And as the temperature goes up the precision of model also increases. The SLD parameters obtained by fitting are reasonable. Because the specific surface area is 2820 m<sup>2</sup>/g closes to Zhou's narrative and the slit width also closes to the diameter of micro pore for the most activated carbon [30-31]. In addition Fig. 8 shows the relation between the energy parameter  $\epsilon_{fs}$  and temperature, and the trend basically

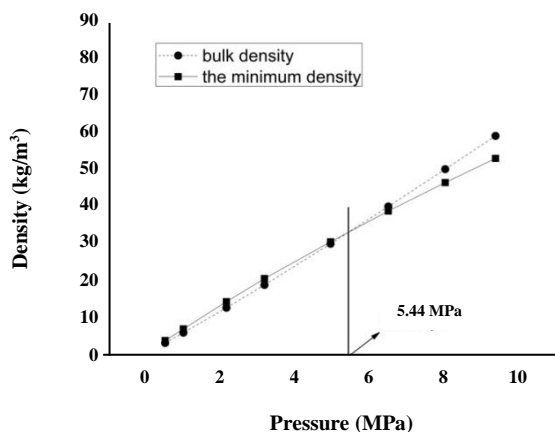


Fig. 9: The intersection of bulk density and the minimum density at 333K.

accords with what has been described by Fitzgerald [32]. Therefore these parameters in SLD model can present the adsorption character of this AX-21 activated carbon with a higher precision. Later on we will use the slit width and specific surface area acquired by fitting with SLD model to calculate density profile and absolute amount of adsorption.

#### Calculate the Absolute Amount of Adsorption

In this Section we will present the application to acquire the absolute adsorption isotherms. According to our method of calculating the absolute amount of adsorption the most important thing is to achieve the thickness of adsorbed phase, which relies on a given density profile for different temperature and pressure. In section 3.1 we have obtained SLD parameters of methane adsorption on AX-21 activated carbon, so we can calculate the density profile by combining Eq. (6) ~Eq. (19) for different temperature and pressure.

As an example we try to get the absolute adsorption isotherm of methane on AX-21 activated carbon at temperature 333K. Firstly we calculate the density profile at each point of pressure to correspond to the pressure point of adsorption isotherm tested by experiment and get all the minimum density of each density profile. And the bulk density for each pressure at 333K is acquired through National Institute of Standards and Technology (NIST). Secondly with fitting we obtain the trend of the minimum density and bulk density varying with pressure and achieve the intersection of two lines (Fig. 9).

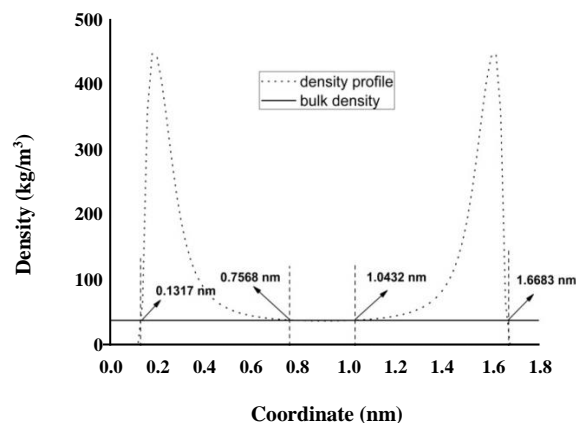


Fig. 10: All the solution of Eq. (5) at 6.5 MPa and 333K.

Then we can find bulk density is less than the minimum density of density profile when the pressure is below 5.44 MPa and more than the minimum density when the pressure is above 5.44 MPa at 333K. So the thickness of adsorbed phase is half of the diameter of pore when the pressure is below 5.44 MPa. While pressure exceeds 5.44 MPa the thickness of adsorbed phase can be determined by solving Eq. (5). Fig. 10 reveals all the solution of Eq. (5) at 6.5 MPa. The solution 0.7568 nm, 1.0432 nm and 1.6683 nm is a possible solution for their value is bigger than the diameter of methane molecular (0.38 nm), and allows for the symmetry of slit pore, so the thickness of adsorbed phase is 0.7568 nm. Similarly we calculate all the thickness of adsorbed phase (Fig. 11) for different pressure and temperature, and then obtain their absolute amount of adsorption (Fig. 12) for Zhou's data [7].

## RESULTS AND DISCUSSION

As we know the density profile is applied to obtain the absolute isotherm, and the absolute amount of adsorption can be achieved with Eq. (2) in theory, but why we don't directly use Eq. (2) with a given density profile? Because so far we can't get the density profile accurately even though we use the most advanced theory method for the moment. And it is difficult to determine the limit of integration of Eq. (2). In addition it will have no association with the precise data of excess adsorption which comes from experiment for the calculation of absolute isotherm with Eq. (2). Hence obtaining the absolute amount of adsorption with Eq. (2) may not be

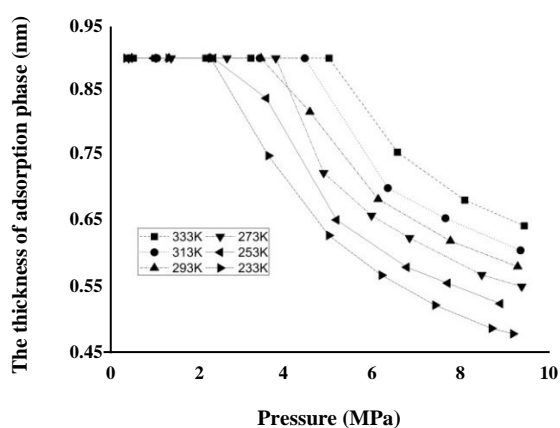


Fig. 11: The thickness of adsorbed phase for 1.8nm slit pore.

the best one. Until now researchers usually calculate the absolute isotherm with Eq. (3), and so do we. Although the pore size distribution of AX-21 is wide and the shape of pore also is various, during the calculation we regard all the pore of AX-21 activated as the same slit pore. Here we adopt a thought of equalization. The SLD can represent the adsorption of methane on the activated carbon with high accurate (Fig. 7), so all the parameters obtained by SLD model represent that the adsorption of methane on AX-21 activated carbon can synthetically describe the adsorption character of this material, then the slit pore and specific surface area achieved by SLD are used to achieve the absolute isotherm. The result can be close to the fact.

In previous content we describe a new method to calculate the absolute amount of adsorption and present the application on the adsorption of methane on AX-21 activated carbon. Finally we acquire the thickness of adsorbed phase (Fig. 11) for 1.8nm slit pore and the absolute sorption isotherms (Fig. 12) with Eq. (3). According to Fig. 11 the thickness of adsorbed phase keeps constant until pressure climbs up to a particular value under the same temperature and then declines with pressure increasing and the thickness also decreases as the temperature declining for 1.8nm slit pore. Because the thickness of adsorbed phase obtained by our method has bearing on the corresponding bulk density, and the bulk density increases with pressure climbing and decreases with temperature increasing. This leads to the thickness obtained by solving Eq. (5) is directly proportional

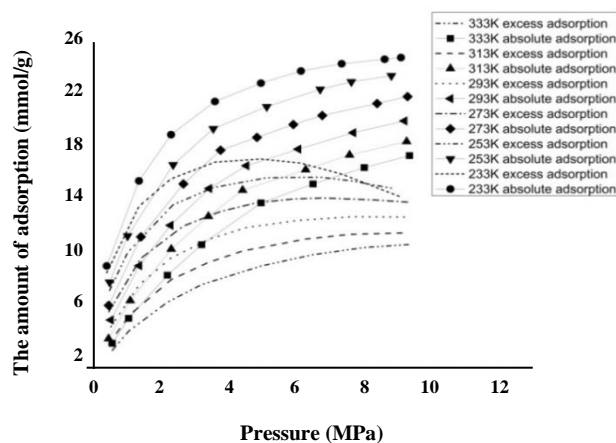


Fig. 12: The absolute amount of adsorption of methane on AX-21 activated carbon.

to the temperature and inversely proportional to the pressure for a specific width of pore if Eq. (5) has solution. If Eq. (5) has no solution means the methane trapped in the pore is in adsorbed state, so the thickness of adsorbed phase is constant (half of the pore diameter).

Obviously the absolute adsorption isotherm (Fig. 12) is monotone increasing and removes the maximum of excess adsorption isotherm. We compare with the absolute amount of adsorption calculated by assuming the volume of adsorbed phase is pore volume and regarding the density of adsorbed phase as the density of liquid and the absolute isotherm of methane on AX-21 comes from Katsuyuki Muratafor 273 and 293K (Fig. 13) [4]. Apparently all these methods to calculate the absolute amount of adsorption can remove the maximum of excess isotherms and can acquire the monotonic adsorption isotherm except the method to regard the pore volume as the volume of the adsorbed phase for 273 and 293K. It seems treating the adsorbed phase as liquid like can achieve the monotone curve, but this method can't apply to calculate the absolute adsorption, because we can't obtain a monotonic adsorption isotherm for a lower temperature (Fig. 14). Furthermore it tells us the adsorbed phase can't be seemed as liquid like for supercritical methane. In addition the pore volume can't be utilized to fulfill the target of gaining the absolute adsorption isotherm as well for it gets barely the appropriate data (Fig. 14) and the definition of adsorbed phase volume also breaks it. Although Katsuyuki Murata's method can



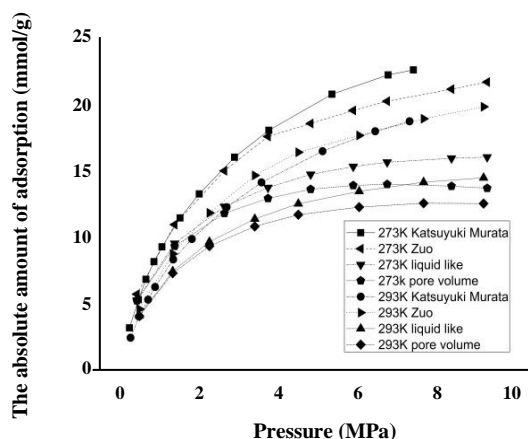


Fig. 13: The absolute amount of adsorption obtained by different method.

calculate the absolute amount of adsorption, the physical background of computation process is undefined. Generally our method not only has a stronger physical mean but also the outcomes achieved by this method also present the reasonable isotherms of absolute adsorption. The rest to appraise the authenticity of our method need serials of experiments or a theory to obtain the absolute amount of methane adsorption on AX-21 activated carbon precisely, which is our direction in the future.

## CONCLUSIONS

In the paper we developed a new method to calculate the absolute amount of adsorption. This method has more clear physical background than the other methods and relies on precise density profile in pore of one material. For the convenience of calculation the mind of equalization is adopted to obtain the same pore size and specific surface area through SLD model represents the excess adsorption isotherm. Compared with the results coming from other methods to calculate the absolute isotherm our result seems very reasonable, besides our method can be applied for large ranges of temperature.

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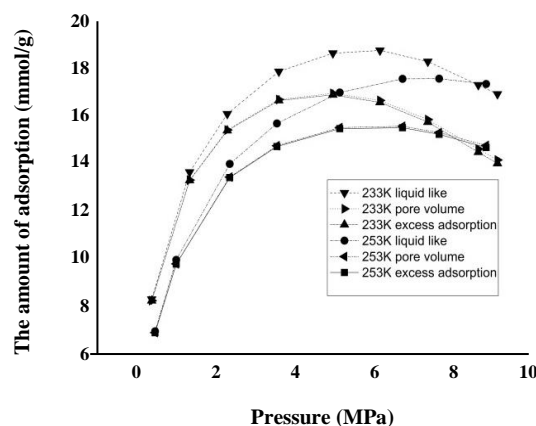


Fig. 14: The amount of adsorption for various situations.

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