

# Better Refined Adsorption Isotherm than BET Equation

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## Abstract

During studying the heat capacity of metals and brightening more than the original Lena's image, the temperature increasing term obtained in binomial expansion is transformed into the adsorption increasing term and thereafter we have derived the total adsorption rate equation with it. In the first layer the quantization does not occur and from 2<sup>nd</sup> layer to n<sup>th</sup> layer the quantization occurs. So as to get the total adsorption rate equation we add the quantized terms of the second to n<sup>th</sup> layers to the non-quantized term of the first layer. All terms are based on the unit surface sites. Instead of the unit surface sites, the new adsorption site term appears in the denominator of the adsorption equation. Hence the adsorption equations come out much better than BET equation. The surface area is also calculated through the integration of the adsorption isotherm equation excluding the first layer adsorption equation from the inflection point to the wanted relative pressure.

## Keywords

Refined BET, Binomial, Transforming, Adsorption Increasing Term, Surface Area, Inflection Point

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## 1. Introduction

We derived the heat capacity equations of metals and then used consistent step multiplication of the appropriate binomial equations [1]. They are fitted to experimental data well [2]. The heat capacity equation (type V) and the adsorption equation (type II) draw sigmoid (S character) lines all together. And they are symmetrical with each other. The measurement gases of heat capacity are hydrogen and helium. The adsorption gases are vapor and nitrogen. The movements of their measurement gases are different. The formers are expansion and the later contraction.

The most important term in the derivation of heat capacity equation was the temperature increasing term,

$g_b \frac{N_n}{N_{n-1} - N_n}$ . In case of adsorption it becomes  $g_a \frac{N_n}{N_{n-1} - N_n}$ . Here  $N_n$  and  $N_{n-1}$  are the total molecules adsorbed at the layers of  $n$  and  $n-1$ . Let us put  $g_a$  which is unit in data fitting as the constant. The constant affects the adsorption equation from starting to ending like other constants. If  $g_a \frac{N_n}{N_{n-1} - N_n}$  is transformed into  $\frac{1}{m}$  power of  $z$  in every derivation of adsorption such as  $g_a \frac{N_n}{N_{n-1} - N_n} = z^{\frac{1}{m}}$  [3], the more advanced adsorption equation than BET eq. comes out. Hence we get the surface area.

## 2. Statistical Modeling of Adsorption Isotherm

Suppose each layer has one binomial equation. And suppose  $N_1$  molecules are adsorbed on  $B$  localized sites of the unit surface layers of the adsorbent and  $\frac{N_2}{m}, \frac{N_3}{m}, \dots, \frac{N_{n-1}}{m}, \frac{N_n}{m}$  molecules on  $\frac{N_1}{m}, \frac{N_2}{m}, \dots, \frac{N_{n-2}}{m}, \frac{N_{n-1}}{m}$  sites made of 1st to  $(n-1)th$  layers in sequence. Here  $m$  is quantization constant. The first adsorption layer has  $D_1$  adsorption energy and the second to  $nth$  layers,  $D_h$ . Hence the adsorption probability on the first layer is  $P_l = W_l \exp(-D_l/k_K t_a)$  and the non-adsorption probability  $1 - W_l \exp(-D_l/k_K t_a)$ . Here  $W_l$  is the adsorption constant of the first adsorption layer.  $t_a$  is similar to  $t_s$  in heat capacity equation. The adsorption constant,  $W_l$  is calculable quantity. It is the expression to combine the rotation and vibration energy of the adsorbed molecules in the first layer.  $k_K$  is similar to  $k_B$  (Boltzmann's constant) [2]. In the combination calculation of the first layer  $N_1$  can take from 0 to  $B$  as variables in sequence. Then the binomial equation of the first layer becomes [1]

$$W_1(B, N_1) = (P_l + 1 - P_l)^B = 1 \cong \sum_{N_1 \leq B} \frac{B!}{(B - N_1)! N_1!} P_l^{N_1} (1 - P_l)^{B - N_1} \quad (1)$$

Next the adsorption probability of from  $N_2$  to  $N_n$  layers is  $P_h = W_h \exp(-D_h/k_K t_a)$  and the non-adsorption probability  $1 - W_h \exp(-D_h/k_K t_a)$ . The binomial equations for from  $N_2$  to  $N_n$  layers are

$$\begin{aligned} W_2\left(N_1, \frac{N_2}{m}\right) &= (P_h + 1 - P_h)^{N_1} = 1 \cong \sum_{\frac{N_2}{m} \leq N_1} \frac{N_1!}{\left(N_1 - \frac{N_2}{m}\right)! \left(\frac{N_2}{m}\right)!} P_h^{\frac{N_2}{m}} (1 - P_h)^{N_1 - \frac{N_2}{m}} \\ &\vdots \\ W_{n-1}\left(\frac{N_{n-2}}{m}, \frac{N_{n-1}}{m}\right) &= (P_h + 1 - P_h)^{\frac{N_{n-2}}{m}} = 1 \cong \sum_{\frac{N_{n-1}}{m} \leq \frac{N_{n-2}}{m}} \frac{\frac{N_{n-2}}{m}!}{\left(\frac{N_{n-2}}{m} - \frac{N_{n-1}}{m}\right)! \left(\frac{N_{n-1}}{m}\right)!} \times P_h^{\frac{N_{n-1}}{m}} (1 - P_h)^{\frac{N_{n-2}}{m} - \frac{N_{n-1}}{m}} \\ &\vdots \\ W_n\left(\frac{N_{n-1}}{m}, \frac{N_n}{m}\right) &= (P_h + 1 - P_h)^{\frac{N_{n-1}}{m}} = 1 \cong \sum_{\frac{N_n}{m} \leq \frac{N_{n-1}}{m}} \frac{\frac{N_{n-1}}{m}!}{\left(\frac{N_{n-1}}{m} - \frac{N_n}{m}\right)! \left(\frac{N_n}{m}\right)!} \times P_h^{\frac{N_n}{m}} (1 - P_h)^{\frac{N_{n-1}}{m} - \frac{N_n}{m}} \end{aligned} \quad (2)$$

Let us multiply Equation (1) and Equation (2) side by side. Then for

$$B \geq N_1 \geq \frac{N_2}{m} \geq \dots \geq \frac{N_{n-1}}{m} \geq \frac{N_n}{m}$$

$$\begin{aligned}
W_{aT} \left( B, N_1, \frac{N_2}{m}, \dots, \frac{N_{n-1}}{m}, \frac{N_n}{m} \right) &= W_1 W_2 \cdots W_{n-1} W_n \cong 1 \\
&\cong \sum_{\frac{N_n}{m} \leq \frac{N_{n-1}}{m}}^{\frac{N_{n-1}}{m}} \cdots \sum_{N_1 \leq B}^B \frac{B! P_l^{N_1} (1-P_l)^{B-N_1} P_h^{N-N_1} (1-P_h)^{N_1 - \frac{N_n}{m}}}{(B-N_1)! \left(N_1 - \frac{N_2}{m}\right)! \cdots \left(\frac{N_{n-1}}{m} - \frac{N_n}{m}\right)! \left(\frac{N_n}{m}\right)!} \\
&= \sum_{\frac{N_n}{m} \leq \frac{N_{n-1}}{m}}^{\frac{N_{n-1}}{m}} \cdots \sum_{N_1 \leq B}^B W_{at}
\end{aligned} \tag{3}$$

$$\text{In the above } N = N_1 + \frac{N_2}{m} + \cdots + \frac{N_{n-1}}{m} + \frac{N_n}{m} \tag{3.1}$$

In Equation (3) the largest term dominates the equation. So the total differential of Equation (3) becomes the zero which requires that the coefficients of all terms should be zero. Hence by using Stirling's approximation we solve the equation,  $W_{at}$ . The first equation (Equation (1)) becomes

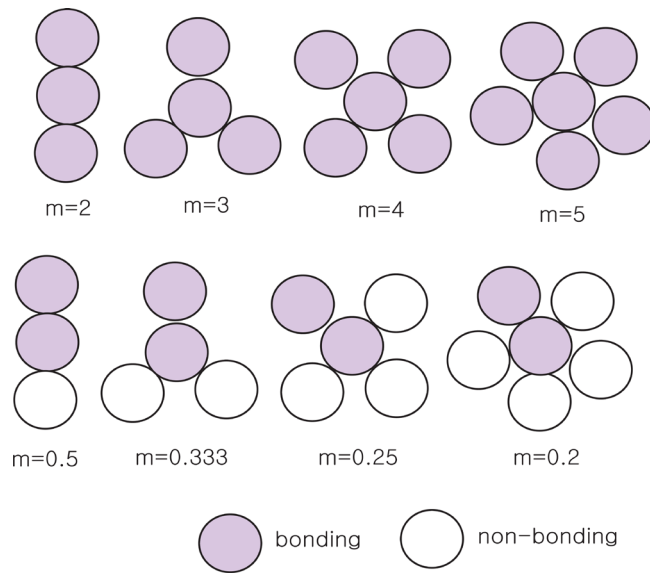
$$\frac{B-N_1}{\beta_a} \left( g_a \frac{N_n}{N_{n-1} - N_n} \right) = N_1 - \frac{N_2}{m} \tag{4}$$

In [4]  $m$  value should be corrected as those in the present figure (**Figure 1**). The constants have three parts of  $m > 1, m = 1, m < 1$ . As we see in **Figure 1**, bonding constants mean quantization. If  $m > 1$ , bonding occurs in many directions. If  $m = 1$  no quantization occur and if  $m < 1$ , the adsorptions are interrupted in many directions. In Equation (4)

$$\beta_a = \frac{W_h}{W_l} \left\{ \exp \frac{-(D_l - D_h)}{k_K t_a} \right\} \left\{ \frac{1 - W_l \exp \frac{-D_l}{k_K t_a}}{1 - W_h \exp \frac{-D_h}{k_K t_a}} \right\} \tag{4.1}$$

$$g_a = 1 - W_h \exp \left( \frac{-D_h}{k_K t_a} \right) = 1 - \exp \frac{-D_h}{k_K t_a} \text{ for } W_h = 1 \tag{4.2}$$

It is possible that  $g_a$  is put as unit.



**Figure 1.** Bonding constant and non-bonding constant in statistic quantization.

The next equations are

$$\begin{aligned}
 \left(N_1 - \frac{N_2}{m}\right) \left(g_a \frac{N_n}{N_{n-1} - N_n}\right) &= \frac{N_2}{m} - \frac{N_3}{m} \\
 &\vdots \\
 \left(\frac{N_{n-3}}{m} - \frac{N_{n-2}}{m}\right) \left(g_a \frac{N_n}{N_{n-1} - N_n}\right) &= \frac{N_{n-2}}{m} - \frac{N_{n-1}}{m} \\
 \left(\frac{N_{n-2}}{m} - \frac{N_{n-1}}{m}\right) \left(g_a \frac{N_n}{N_{n-1} - N_n}\right) &= \frac{N_{n-1}}{m} - \frac{N_n}{m} \quad n = 2, 3, 4, \dots
 \end{aligned} \tag{5}$$

In Equations (4) and (5) let us put  $g_a \frac{N_n}{N_{n-1} - N_n} = z^{\frac{1}{m}}$ , then  $z = p/p_0$  which is same as Equation (9) of [5] solved by using the chemical potential

$$\begin{aligned}
 \frac{B - N_1}{\beta_a} z^{\frac{1}{m}} &= N_1 - \frac{N_2}{m} \\
 \left(N_1 - \frac{N_2}{m}\right) z^{\frac{1}{m}} &= \frac{N_2}{m} - \frac{N_3}{m} \\
 &\vdots \\
 \left(\frac{N_{n-3}}{m} - \frac{N_{n-2}}{m}\right) z^{\frac{1}{m}} &= \frac{N_{n-2}}{m} - \frac{N_{n-1}}{m} \\
 \left(\frac{N_{n-2}}{m} - \frac{N_{n-1}}{m}\right) z^{\frac{1}{m}} &= \frac{N_{n-1}}{m} - \frac{N_n}{m}
 \end{aligned} \tag{6}$$

In Equation (6) add side by side and rearrange

$$\frac{B - N_1}{\beta_a} \left( \frac{z^{\frac{1}{m}} - z^{\frac{n}{m}}}{1 - z^{\frac{1}{m}}} \right) = N_1 - \frac{N_n}{m} \tag{7}$$

In Equation (6) multiple side by side and rearrange

$$\frac{B - N_1}{\beta_a} z^{\frac{n-1}{m}} = \frac{N_{n-1}}{m} - \frac{N_n}{m} \tag{8}$$

We solve Equation (8) with  $g_a \frac{N_n}{N_{n-1} - N_n} = z^{\frac{1}{m}}$  in order to eliminate  $N_{n-1}$

$$\frac{B - N_1}{\beta_a} \frac{1}{g_a} z^{\frac{n}{m}} = \frac{N_n}{m} \tag{9}$$

We solve Equation (7) with Equation (9) in order to eliminate  $N_n$

$$\frac{N_1}{B} = \frac{\frac{z^{\frac{1}{m}} - z^{\frac{n}{m}}}{1 - z^{\frac{1}{m}}} + \frac{z^{\frac{n}{m}}}{g_a}}{\beta_a + \frac{z^{\frac{1}{m}} - z^{\frac{n}{m}}}{1 - z^{\frac{1}{m}}} + \frac{z^{\frac{n}{m}}}{g_a}} \tag{10}$$

Equation (10) represents the adsorption amount of the first layer. It is Langmuir equation. The quantization values ( $m$ ) and the numbers of the adsorption layer ( $n$ ) are influential on the determination of  $N_1$ . All values

of the parameters ( $\beta_a$ ,  $g_a$ ,  $n$ ,  $m$ ) directly participate in the determination of  $N_1$  and following  $N$ . The value of  $g_a$  is much influential on the determination of the last term ( $z^{\frac{n}{m}}$ ). But it does not much increase or decrease of  $N_1$  since it exists in the denominator and nominator. At  $m=1$  it becomes

$$\frac{N_1}{B} = \frac{\frac{z-z^n}{1-z} + \frac{z^n}{g_a}}{\beta_a + \frac{z-z^n}{1-z} + \frac{z^n}{g_a}} \quad (11)$$

Equation (11) is the same as Equation (10) obtained by using chemical potential in [1]. Therefore the total adsorption amount per unit surface ( $B$ ), that is, the adsorption isotherm for from first layer to the last ( $n$ ) layer becomes by using Equations (6) and (10) as follows

$$\begin{aligned} \frac{N}{B} &= \frac{N_1}{B} + \frac{N_2}{mB} + \frac{N_3}{mB} + \dots + \frac{N_{n-1}}{mB} + \frac{N_n}{mB} \\ &= \frac{1}{B} \left\{ N_1 + \left( \frac{N_2}{m} - \frac{N_3}{m} \right) + 2 \left( \frac{N_3}{m} - \frac{N_4}{m} \right) + \dots + (n-2) \left( \frac{N_{n-1}}{m} - \frac{N_n}{m} \right) + (n-1) \frac{N_n}{m} \right\} \\ &= \frac{a}{\beta_a + a} \left\{ 1 + \frac{1}{a} \left( \frac{\frac{z}{z^m} - \frac{z^n}{z^m}}{\left( 1 - z^{\frac{1}{m}} \right)^2} + \frac{n-1}{g_a} z^{\frac{n}{m}} \right) \right\} \end{aligned} \quad (12)$$

In the above

$$a = \frac{\frac{1}{z^m} - \frac{z^n}{z^m}}{1 - z^{\frac{1}{m}}} + \frac{z^{\frac{n}{m}}}{g_a} \quad (12.1)$$

And the total adsorption rate is a linear function of  $z$  made of four constants ( $\beta_a$ ,  $g_a$ ,  $n$ ,  $m$ ). The equation draws BET-like lines and fits BET type experimental data well. At  $m=1$  it becomes

$$\frac{N}{B} = \frac{1}{B} (N_1 + N_2 + N_3 + \dots + N_{n-1} + N_n) = \frac{a'}{\beta_a + a'} \left\{ 1 + \frac{1}{a'} \left( \frac{z^2 - z^n}{(1-z)^2} + \frac{n-1}{g_a} z^n \right) \right\} \quad (13)$$

In the above

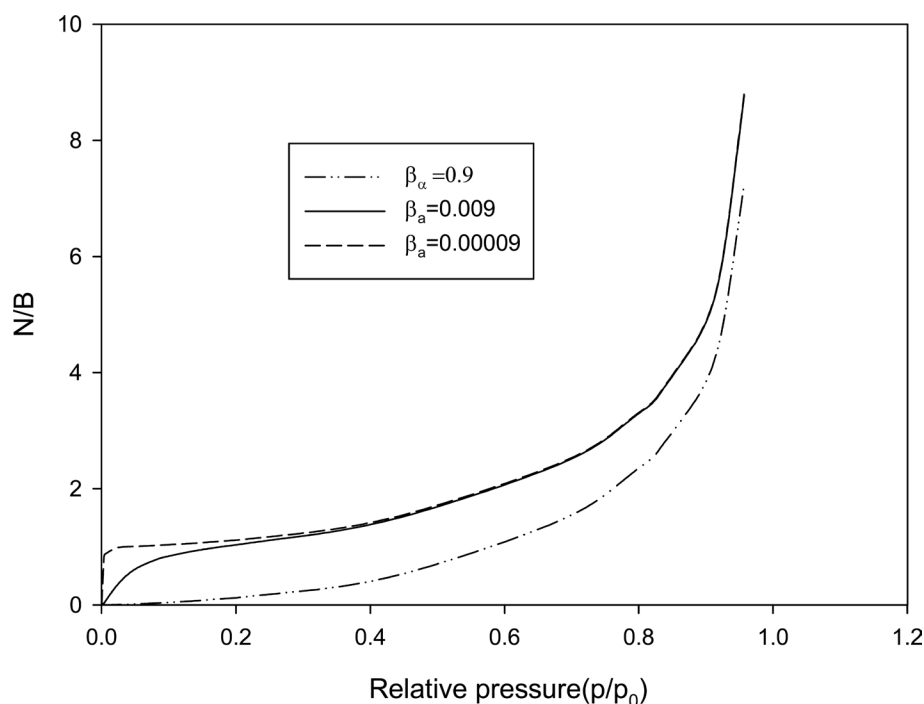
$$a' = \frac{z - z^n}{1 - z} + \frac{z^n}{g_a} \quad (13.1)$$

If the measurement gas is nitrogen, the general empirical formulae,  $A_m = 1.091 \left( \frac{M}{\rho N} \right)^{\frac{2}{3}} \times 10^{16}$  is introduced into.  $S = \frac{x_m}{M} \times N \times A_m \times 10^{-20}$  to get the specific surface area of the adsorbate,  $S$  [6]. Then  $M$  is the molecular weight of nitrogen and  $\rho$  density of nitrogen and  $N$  Avogadro number, Hence from empirical formulae  $A_m = \text{\AA}^2/\text{number}$  is used. The monolayer capacity,  $x_m$  should also be substituted by the value of the integration of Equation (12) subtracted by the surface adsorption isotherm ( $N_1/B$ ).

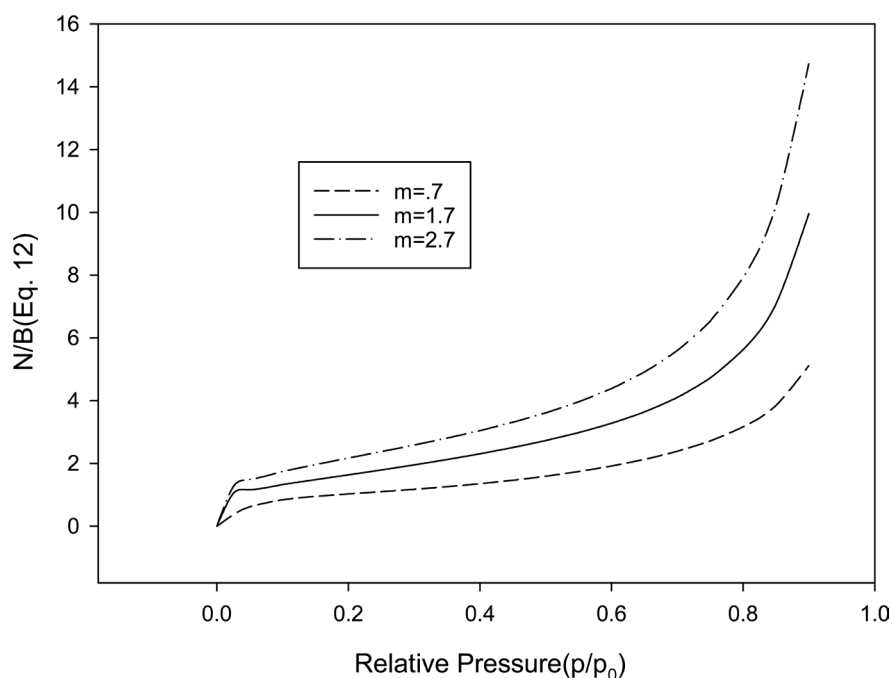
### 3. Result and Discussion

The base of Equations ((10) and (12)) is  $\beta_a + a$ . So we may use the word, the rate without considering dimension. It affects the equation totally. Figure 2 shows the total adsorption rate according to the values of  $\beta_a$ . In

accordance with the values of  $z$  approaching units, the total adsorption rates approach closely with one another. This seems to mean that the adsorption heat of the first layer is same as those of  $2 \sim n$  layers. We call  $m$  the quantization values. It seems to have same notion as the quantization appears in quantum mechanism. We are dealing statistical quantization which should exist in statistics. We can discern them, three cases.  $m > 1, m = 1$  and  $m < 1$ . The cases of  $m > 1$  and  $m = 1$  explain bonding and  $m < 1$  explains the existence of the interruptions for bonding. **Figure 3** explains the increase of the adsorption rate according to  $m$  values.

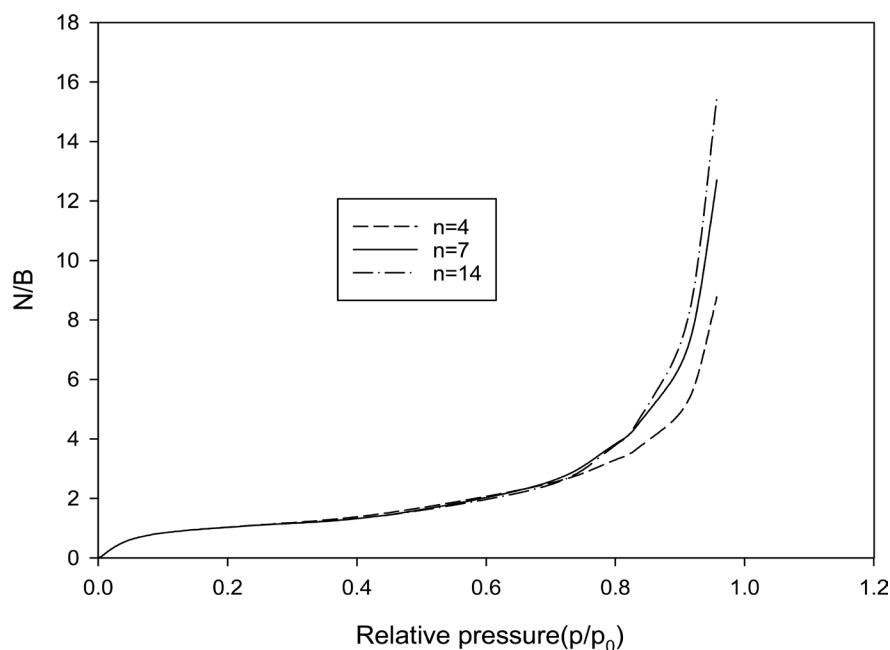


**Figure 2.** Theoretical adsorption isotherm curve, Equation (12) ( $m = 0.7, n = 4, g_a = 0.5$ ) with respect to  $\beta_a$  values.

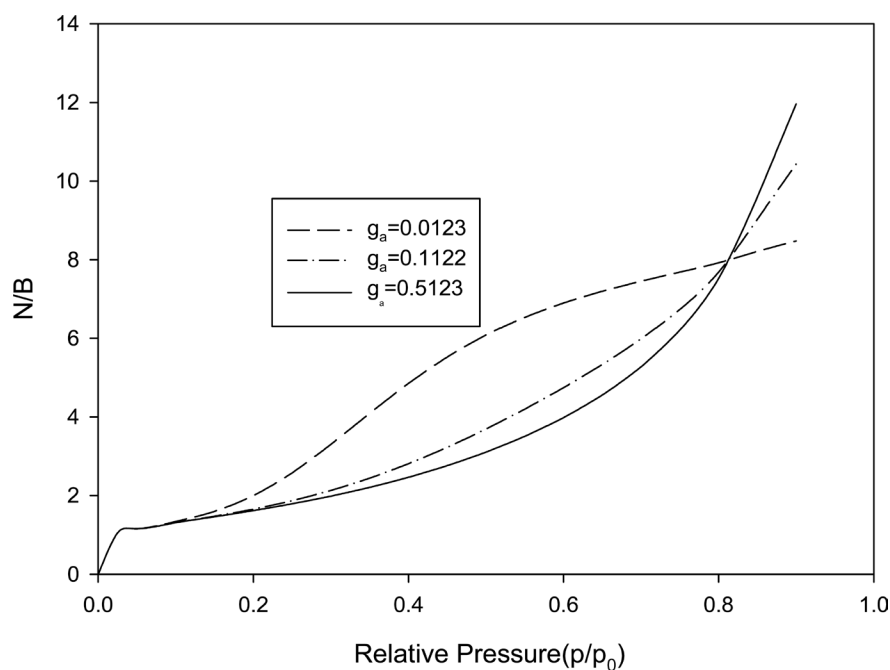


**Figure 3.** Theoretical adsorption isotherm curve, Equation (12) ( $n = 4, \beta_a = 0.00901, g_a = 1.0$ ) with respect to  $m$  values.

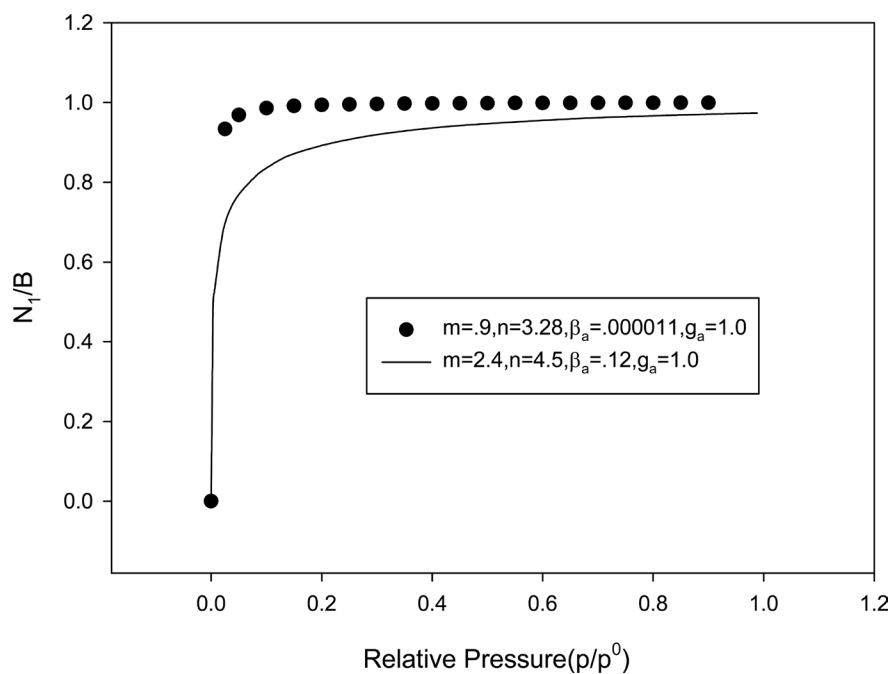
Less  $m$  than unit seem to interrupt the bonding. **Figure 4** represents the total adsorption rates according to  $n$  values. At less  $z$  than 0.5 the isotherms show the same adsorption rates. The constant  $g_a$  showed in **Figure 5** should be positive. When  $g_a = 0.5123$  and  $g_a = 0.1122$ , the constants draw the type II isotherm, but at  $g_a = 0.0123$  the different type (type IV) of the isotherm appear. **Figure 6** shows  $N_1/B$  with respect to the relative pressure like Langmuir's lines which can't become unit even if  $a$  is very large or  $\beta_a$  much smaller. The parameter values of **Figure 6** come from **Figure 7** and **Figure 8**. According to the above variations we optimized two kinds of the experimental adsorption isotherm data showed in **Figure 7** [6] and **Figure 8** [7] using trial and error method. The experimental data of **Figure 7** are obtained from the Figures 2-10 of [6]. The



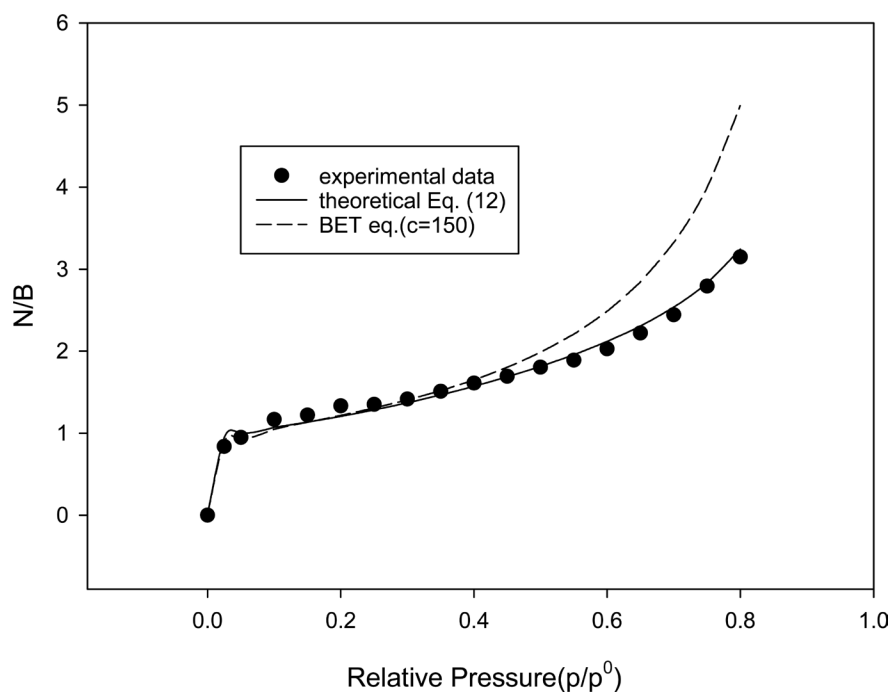
**Figure 4.** Theoretical adsorption isotherm curves, Equation (12) ( $\beta_a = 0.009$ ,  $g_a = 0.5$ ,  $m = 0.7$ ) with respect to  $n$  values.



**Figure 5.** Theoretical adsorption isotherm curve, Equation (12) ( $m = 1.7$ ,  $n = 8$ ,  $\beta_a = 0.009$ ) with respect to  $g_a$  values.



**Figure 6.** Theoretical adsorption isotherm of the first layer using Equation (10) including experimental constants of **Figure 7** and **Figure 8**.



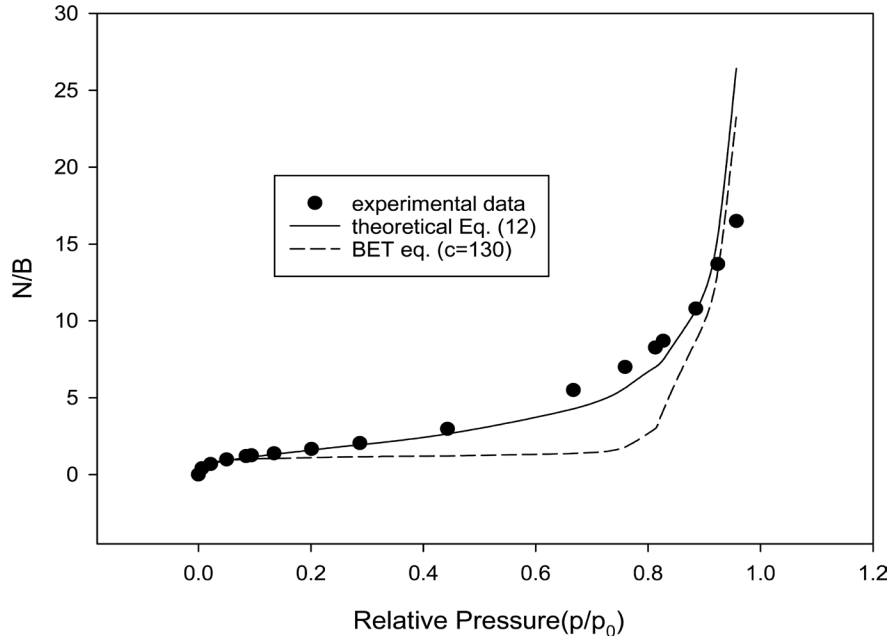
**Figure 7.** Theoretical adsorption isotherm, Equation (12) ( $m = 0.9$ ,  $n = 3.28$ ,  $\beta_a = 0.000011$ ,  $g_a = 1.0$ ) with BET equation ( $c = 150$ ) and experimental nitrogen adsorption at  $-196^\circ$  on non-porous samples of silica and alumina [6].

experimental data are fitted to Equation (12) well. As we see in **Figure 7** and **Figure 8**, BET isotherms there can't imitate the experimental data except for beginning.

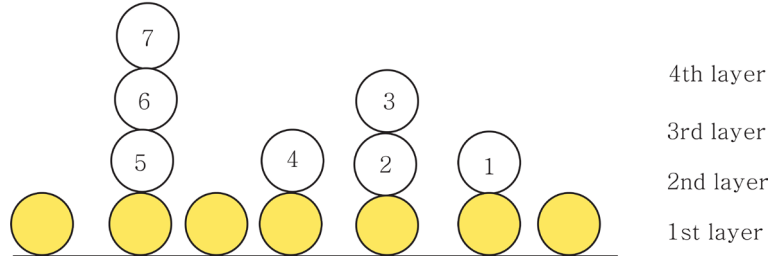
Equation (13) can be used in the data fitting with  $m = 1.0$  and  $g_a = 1.0$ . Its quality is poor.

What is the catalyst? As we see **Figure 9**, 1, 2, 3, 4, 5, 6 and 7 molecules can function as the catalyst. That is, the molecules of the surface adsorption layer can't function like the catalyst. Because they use much





**Figure 8.** Theoretical adsorption isotherm curve, Equation (12) ( $m = 2.4$ ,  $n = 4.5$ ,  $\beta_a = 0.12$ ,  $g_a = 1.0$ ) with BET equation ( $c = 130$ ) curve and experimental water adsorption at 25° on cross-linked polystyrene sulfuric acid resin [7].



**Figure 9.** Real adsorption molecules to get the surface area (numbered rings).

energy in order to hold the surface. So they are not active. The molecules which lie on the surface layer adsorption molecules which hold the surface, can function as the real catalyst. Therefore in Equation (12)

$$\frac{1}{\beta_a + a} \left\{ \frac{\frac{2}{z^m} - \frac{n}{z^m}}{\left(1 - z^m\right)^2} + \frac{n-1}{g_a} z^{\frac{n}{m}} \right\} \text{ part must work in the adsorption reaction. Hence the real adsorption isotherm}$$

equation becomes

$$\frac{N_{real}}{B} = \frac{1}{\beta_a + a} \left\{ \frac{\frac{2}{z^m} - \frac{n}{z^m}}{\left(1 - z^m\right)^2} + \frac{n-1}{g_a} z^{\frac{n}{m}} \right\} \quad (14)$$

If this equation is integrated from the inflection point ( $z_i$ ) to each relative pressure ( $p/p_0$ ), we get the mono-area capacity ( $S_m$ ) with respect to the relative pressure ( $p/p_0$ ). **Table 1** and **Table 2** include those. Then

**Table 1.**  $S_m$  (mono-area capacity) and  $S$  (surface area) for **Figure 7**.

$p/p_0$ integration interval Inflection point ( $z_i = 0.573$ )	$S_m$ for <b>Figure 7</b> ( $m = 0.9, n = 3.28, \beta_a = 0.000011, g_a = 1.0$ ) $S_m = \int_{z_i}^{z_m} \frac{N_{real}}{B} dz$	$S$ ( $m^2/g$ ) for <b>Figure 7</b> = Surface Area of Catalyst, Nitrogen
0.573 - 0.6	0.000042	0.2927
0.573 - 0.7	0.000199	1.3869
0.573 - 0.8	0.000355	2.4741
0.573 - 0.9	0.000512	3.5683

**Table 2.**  $S_m$  (mono-area capacity) and  $S$  (surface area) for **Figure 8**.

$p/p_0$ integration interval Inflection point ( $z_i = 0.26$ )	$S_m$ for <b>Figure 8</b> ( $m=2.4, n=4.5, \beta_a = 0.12, g_a = 1.0$ ) $S_m = \int_{z_i}^{z_m} \frac{N_{real}}{B} dz$	$S$ ( $m^2/g$ ) for <b>Figure 8</b> = Surface Area of Catalyst, Water
0.26 - 0.3	0.00175	5.5968
0.26 - 0.4	0.00615	19.6690
0.26 - 0.5	0.01050	33.5812
0.26 - 0.6	0.01490	47.6533
0.26 - 0.7	0.01930	61.6665
0.26 - 0.8	0.02372	76.0261
0.26 - 0.9	0.02810	89.8698

the surface area for the catalyst obtained from the equation becomes  $S(m^2/g) = (S_m/M) \cdot N \cdot A_m \times 10^{-20}$  with  $A_m = 16.2 \text{ \AA}^2$  per number for nitrogen and  $A_m = 0.59 \times 16.2 \text{ \AA}^2$  per number for water (Table 2.12) [6] by substituting  $x_m$  in the equation of (2.60) of the reference [6] by  $S_m = \int_{z_i}^{z_m} \frac{N_{real}}{B} dz$  in which  $z_i$  = inflection point

and  $z_m$  = optional  $z$  value after the inflection point. In the above equation  $M$  is the molecular weight (g) per g-mole and  $N$  Avogadro number per g-mole.

Then the inflection points are obtained by Secant method [8] through the program showed in **Appendix 1**. Specific surface areas are changed according to the relative pressures. These are showed in **Table 1** and **Table 2** precisely. The integrations with respect to  $z$  values give the total adsorption site numbers of the adsorbate. Before the inflection point the specific surface area of the adsorbent is not counted as a catalyst since it makes the strong surface film [9]. The adsorption rate increases consistently after the inflection point. The values of  $n$  of **Figure 7** and **Figure 8** match the range of the reference of BET [10]. The completion of  $N_1$  goes with the completion of  $N$  to the end as we see in **Figure 6** and its equation. But from the inflection point the plugging of  $N_1/B$  may begin characteristically.

We have felt intimately that the adsorption molecules of more than 2<sup>nd</sup> layers lie down the first layer molecules softly since the small quantity of adsorption molecules control the drawing and the surface area of numerical number.

Our study have realized the saying that “After considerable work on the theory, Hill (1946) formed the opinion that any future improvement on it must be in the form of refinement rather than a modification on the basic theory” [11] [12].

## 4. Conclusion

The total adsorption rate equations closely related with the past references are derived correctly and the figures according to four constants ( $m, n, \beta_a, g_a$ ) are also considered to describe BET-like figures (type II) well. The quantization constants are useful in deriving the adsorption equations. In order to calculate the surface area of

the catalysts, the total adsorption equations excluding the first layer adsorption equation and their inflection points obtained are used appropriately. They fit the experimental data well.

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## Appendix 1

/\*--Finding zero by Secant method [8] to get inflection point from Eq. (12). with c++ and c languages \*/

```
#include<iostream>
using namespace std;
#include<stdio.h>
#include<math.h>
#include<conio.h>
float eval_f(float x); //evaluation of f(x)
float fprime(float x1,float x2); //diff. of f(a)

void main()
{ float x1,x2,xn,e;
  int i=0;
  printf("\nType initial point: ");
  scanf("%f", &x1);
  printf("\nType second point: ");
  scanf("%f",&x2);
  printf("\nType acceptable error interval in y: ");
  scanf("%f", &e);

  i=0;
  do
  { xn=x1-eval_f(x1)/fprime(x1,x2);
    x1=x2;
    x2=xn;
    printf("\n%3dth Iteration Root :%f <with error %f >\n",
      ++i,xn,fabs(eval_f(xn)));
    getch();
  } while(fabs(eval_f(xn))> e);
}

float eval_f(float x)
{ float b;
  //cout<<"x="<<x<<endl;
  double bc;
  double bb,bb1,bb2,cc,dd,dd1,dd2,dd3,ee,ee1,ee2,ff,ff1,ff2;
  double aa,aa1,aa2,ba1,ba2,ba3,ccc1,ccc2,cc1,cc2,cc3,cc4,cc11,cc12;
  const double b1=.000091,ga=.983,an=10.0,am=.64;
  double ad21,ad22,ad23;
  bb=pow(x,(1./am))-pow(x,(an/am));
  bb1=(1./am)*pow(x,(1./am)-1.)-(an/am)*pow(x,(an/am-1.));
  bb2=(1./am)*(1./am-1.)*pow(x,(1./am)-2.)-(an/am)*(an/am-1.)*pow(x,(an/am-2.));
  ccc1=-(1./am)*pow(x,1./am-1.);
  ccc2=-(1./am)*(1./am-1.)*pow(x,1./am-2.);
  cc1=pow((1.-pow(x,1./am)),1.);
  cc2=pow((1.-pow(x,1./am)),2.);
  cc3=pow((1.-pow(x,1./am)),3.);
  cc4=pow((1.-pow(x,1./am)),4.);
  dd=pow(x,(an/am))/ga;
  dd1=(an/am)*pow(x,((an/am)-1.))/ga;
  dd2=(an/am)*(an/am-1.)*pow(x,((an/am)-2.))/ga;
```

---

```

ee=pow(x,2./am)-pow(x,an/am);
ee1=(2./am)*pow(x,(2./am)-1.)-(an/am)*pow(x,(an/am)-1.);
ee2=((2./am)*(2./am-1.)*pow(x,(2./am)-2.)-(an/am)*(an/am-1.)*pow(x,(an/am-2.));
ff=((an-1.)/ga)*pow(x,an/am);
ff1=((an-1.)/ga)*(an/am)*pow(x,(an/am)-1.);
ff2=((an-1.)/ga)*(an/am)*(an/am-1.)*pow(x,(an/am)-2.);

aa=bb*cc1+dd;
aa1=bb1*cc1+(-1)*cc2*ccc1*bb+dd1
aa2=bb2*cc1+(-1)*cc2*ccc1*bb1+(-1)*(-2)*cc3*ccc1*ccc1*bb+(-1)*ccc2*cc2*bb+(-1)*bb1*cc2*ccc1+dd2;

ba1=pow((b1+aa),-1);
ba2=pow((b1+aa),-2);
ba3=pow((b1+aa),-3);

ad21=aa2*ba1+(-1)*ba2*aa1*aa1+(-1)*(-2)*ba3*aa1*aa1*aa+(-1)*aa2*ba2*aa+(-1)*aa1*aa1*ba2;

ad22=ee2*cc2*ba1+(-2)*cc3*ccc1*ee1*ba1+(-1)*ba2*aa1*ee*cc2+(-2)*(-3)*cc4*ccc1*ccc1*ee*ba1+(-2)*ccc
2*cc2*ee*ba1+(-2)*ee1*cc3*ccc1*ba1+(-2)*(-1)*ba2*aa1*cc3*ccc1*ee+(-1)*(-2)*ba3*aa1*aa1*ee*cc2+(-1)*
aa2*ba2*ee*cc2+(-1)*ee1*ba2*aa1*cc2+(-1)*(-2)*cc3*ccc1*ba2*aa1*ee1;

ad23=ff2*ba1+(-1)*ba2*aa1*ff1+(-1)*(-2)*ba3*aa1*aa1*ff+(-1)*aa2*ff*ba2+(-1)*ff1*ba2*aa1;
b=ad21+ad22+ad23;
return(b);
}
float fprime (float x1,float x2)
{ float b6;
b6=(eval_f(x2)-eval_f(x1))/(x2-x1);
return(b6);
}

```