Ecuación BET

M_i = número de sitios recubiertos a una profundidad de i moléculas (i layers), $M_i=x^i c M_0$

$$x = \frac{k_{ap}}{\nu \exp\left(-\frac{\varepsilon_V}{kT}\right)} = \frac{k_a}{k_{d,i\geq 2}} p$$

$$c = exp\left(\frac{\varepsilon - \varepsilon_V}{k_B T}\right)$$

Volumen total adsorbido

$$V = \sum_{i=1}^{n} V_i \propto \sum_{i=1}^{n} iM_i$$

Volumen adsorbido en una monocapa:

$$V_m \propto M = M_0 + \sum_{i=1}^{n} M_i$$

Y

$$\frac{V}{V_m} = \frac{\sum_i iM_i}{M_o + \sum_i M_i} = \frac{c\sum_i ix^i}{1 + c\sum_i x^i}$$

finalmente,

$$\frac{V}{V_m} = \frac{cx}{(1-x)[1+(c-1)x]}$$

Que se puede reescribir como:

$$\frac{1}{V}\frac{x}{1-x} = \frac{c-1}{cV_m}x + \frac{1}{cV_m}$$

Entonces al grafica (1/V)[x/(1-x)] vs x debe dar una línea recta,

$$pendiente = m = \frac{c-1}{cV_m}$$

$$ordenada\ al\ origen = b = \frac{1}{cV_m}$$

Entonces:

$$V_m = \frac{1}{m+b}, \quad c = \frac{m}{b} + 1$$

Además

$x = \frac{p}{p^0}$

Que es la presión relativa a la presión de saturación. La ecuación de BET describe el volumen de gas adsorbido a diferentes valores de p/p^0 en términos V_m y c.

Figure 9.9a is a plot of some actual experimental data showing the volume of N_2–

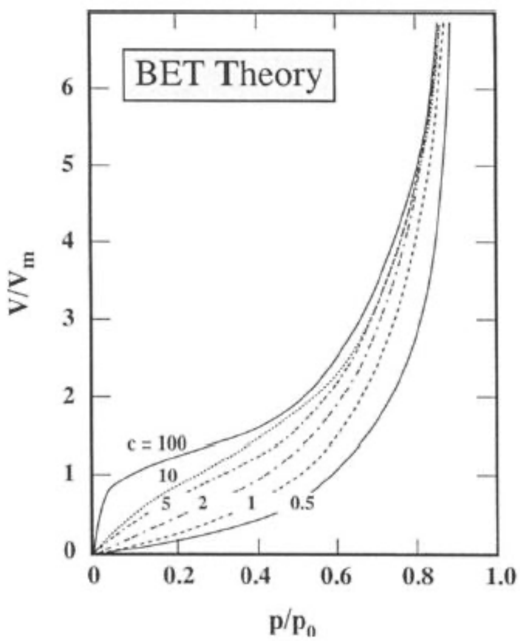

FIG. 9.8 Plots of V/V_m versus p/p_0 for several values of the parameter c, calculated according to the BET theory by Equation (71).

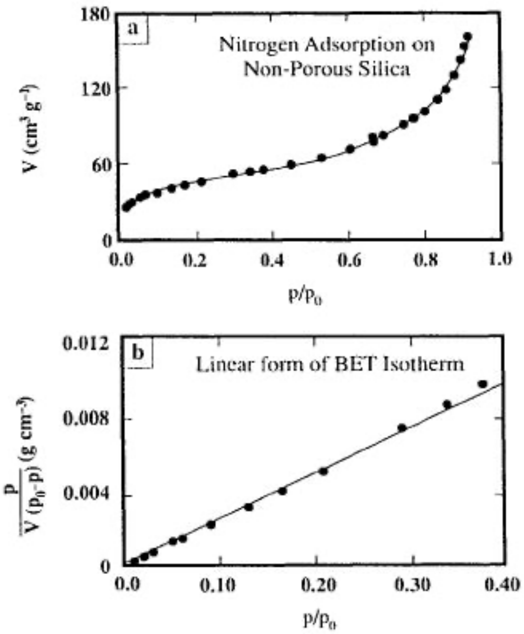

FIG. 9.9 Nitrogen adsorption on nonporous silica at 77K. (a) volume per gram (in cm^3 per gram at STP) versus p/p_0; and (b) according to the linear form of the Brunauer-Emmett-Teller equation (Equation (74)). (Data from D. H. Everett, G. D. Parfitt, K. S. W. Sing, and R. Wilson, *J. Appl. Chem. Biotechnol.*, **24**, 199 (1974).)

En este ejemplo, valor de la pen diente = 0.0257 g/cm^3 a STP

Ordenada al origen=$2.85x10^{-4}$ g/cm^3 a STP

$$V_m = \frac{1}{(257 + 2.85)x10^{-4}} = 38.5 \frac{cm^3}{g}\, a\, STP$$

$$c = \frac{257x10^{-4}}{2.85x10^{-4}} + 1 = 91.2$$

De la relación

$$V_m = \left(\frac{n}{w}\right)_{sat} (22414 \frac{cm^3}{mol})$$

Tenemos:

$$A_{sp} = \frac{V_m N_A \sigma^0}{22414}$$

En este caso

$$A_{sp} = \frac{(38.5cm^3/g)x6.02x10^{23}mol^{-1}x16x10^{-16}cm^2}{22414\, cm^3/mol} = 165.4x10^4 cm^2/g = 165.4m^2/g$$