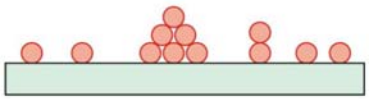
2. The BET model

Brunauer, Emmett és Teller

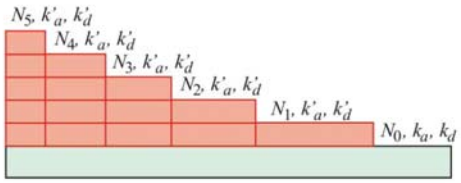
*Planar surface

*Binding sites of equal energy

*Multilayer coverage



reality



model

$$A_{(gas)} + S \rightleftharpoons AS \qquad k_a N_0 p = k_d N_1$$

$$A_{(gas)} + AS \rightleftharpoons A_2S \qquad k'_a N_1 p = k'_d N_2$$

$$A_{(gas)} + A_2S \rightleftharpoons A_3S \qquad k'_a N_{i-1} p = k'_d N_i$$

etc.

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$$k_a \propto \exp\frac{E_a}{RT} \qquad k'_a \propto \exp\frac{E_L}{RT}$$

$$n^S = \frac{n_m \cdot C \cdot \frac{p}{p_o}}{\left(1-\frac{p}{p_o}\right)\cdot\left[1+(C-1)\frac{p}{p_o}\right]}$$

$$C = e^{\frac{(E_a - E_L)}{RT}}$$

C depends on the quality and shows the rel. strength of the interaction

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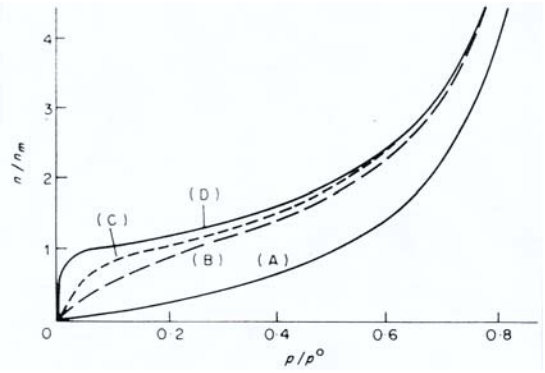
A mathematical feature of the BET model



(A) $C = 1$
(B) $C = 11$
(C) $C = 100$
(D) $C = 10000$

$C > 2$ → Type II
$0 < C < 2$ → Type III

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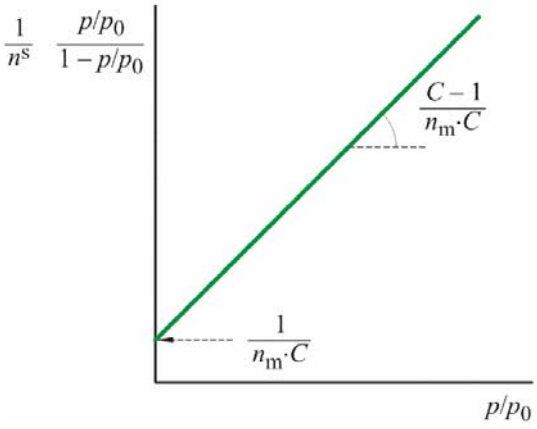
A linearized form

$$\frac{1}{n^s} \cdot \frac{\frac{p}{p_0}}{1 - \frac{p}{p_0}} = \frac{1}{n_m C} + \frac{C - 1}{n_m C} \cdot \frac{p}{p_0}$$



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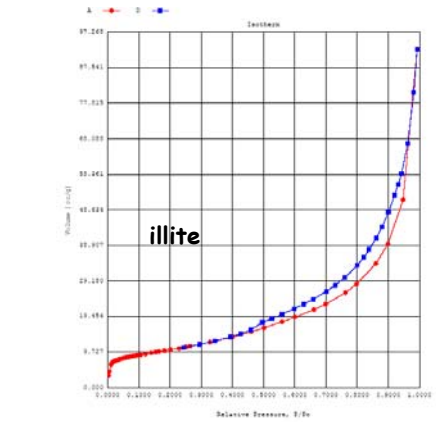

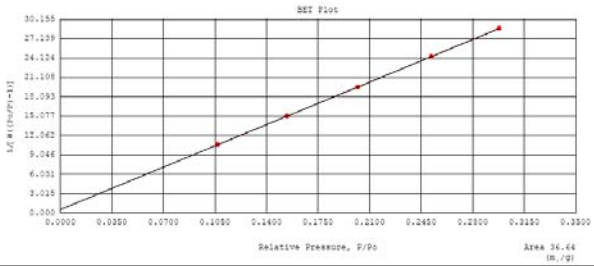

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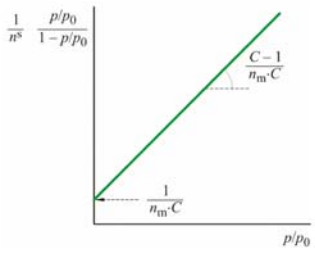
Single point BET



$C \geq 80$

$$\frac{1}{V} \cdot \frac{\frac{p}{p_0}}{1-\frac{p}{p_0}} = \frac{1}{V_m C} + \frac{C-1}{V_m C} \cdot \frac{p}{p_0} \approx \frac{1}{V_m} \cdot \frac{p}{p_0}$$

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Summary of the BET model

Multilayer adsorption
- Planar surface
- Energetically homogeneous binding sites
- Infinite number of adsorbed layers is possible
- First layer: heat of adsorption
- All the other layers: heat of condensation
- The adsorption is localized
- No exchange between the layers

works: *isotherms of Types II and IV*

nonporous disperse systems

macroporous systems

d>2 nm mesoporous systems

Rule of thumb: $0.05 < p/p_0 < 0.3$

Strictly speaking it can not be used for microporous systems!!!

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Interpretation of the fitted parameters

1. Derivation of specific surface area from monolayer capacity

$$S_A = n_m \cdot N_A \cdot a_s \qquad \frac{m^2}{g}$$

RESTRICTIONS!!!!

Monolayer capacity

Avogadro's number

Area occupied by a single adsorbent

1) (Most often) N_2, 77 K
2) Initial part of the isotherm (BET: p/p_0=0.05-0.35)
1) n_m from the linear plot of minimum 5 measured points
2) a_s=0.162 nm^2

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