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Extension of the *Hüttig* Isotherm on Mixed Gas Adsorption

Short Communication

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Hüttig's theory was extended for mixed gas adsorption. The derived equation is the same as the one that has been obtained by *Gonzalez* and *Holland* for bilayer adsorption.

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Erweiterung der Hüttig-Isotherme für Gasmischungen (Kurze Mitteilung)

Die Theorie von *Hüttig* wurde auf gemischte Gase ausgedehnt. Die dabei abgeleitete Gleichung ist dieselbe wie die von *Gonzalez* und *Holland* für Zweischichtadsorption.

The increased use of solid adsorbents in separation processes has led to the need for methods of predicting the equilibria of multicomponent mixtures from the knowledge of the adsorption equilibrium for pure components. The best known analytical form of an adsorption isotherm is the *Langmuir* equation extended by *Markham* and *Benton*[1] to monolayer mixed gas adsorption. *Brunauer*, *Emmett* and *Teller*[2] adapted *Langmuirs* theory to multilayer adsorption. *Hill*[3] followed by *Arnold*[4] proposed extension of the *BET* equations for the description of multicomponent adsorption. *Hüttig*[5] proposed a slightly different model in his extension of the *Langmuir* equation on multilayer adsorption. The only essential difference is whether or not the molecules adsorbed in the higher layers are capable of preventing the evaporation of underlying molecules. According to *BET* the desorption is completely impeded while *Hüttig* considers that the presence of higher layers is of no effect on the evaporation from underlying layers.

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The expression obtained by *Hüttig* for the multilayer adsorption is given by

$$\Theta = \frac{ap}{1+ap}(1+bp) \tag{1}$$

where Θ is surface coverage, p pressure, a and b are constants.

Following the *Hüttig* mechanism we can write for first layer and i-th component

$$a_{i,1}p_i\left(1-\sum_{i=1}^{n}\Theta_{i,1}\right)=\Theta_{i,1} \tag{2}$$

where

$$a_{i,1}=\frac{K'_{i,1}}{K''_{i,1}}$$

with $K'_{i,1}$, $K''_{i,1}$-rate adsorption and desorption respectively; for second

$$a_{i,2}p_i\left(\sum_{i=1}^{n}\Theta_{i,1}-\sum_{i=1}^{n}\Theta_{i,2}\right)=\Theta_{i,2} \tag{3}$$

and for m-th

$$a_{i,m}p_i\left(\sum_{i=1}^{n}\Theta_{i,m-1}-\sum_{i=1}^{n}\Theta_{i,m}\right)=\Theta_{i,m} \tag{4}$$

Now, we apply the *BET* assumption

$$E_2=E_3=\ldots=E_m \tag{5}$$

and we can express

$$a_{i,2}=a_{i,3}=a_{i,4}=\ldots.=a_{i,m}=b_i. \tag{6}$$

Adsorption i-th component in the first layer from equation (2)-(6) is

$$\Theta_{i,1}=\frac{a_i p_i}{1+\sum_{i=1}^{n}a_i p_i} \tag{7}$$

in the second

$$\Theta_{i,2} = \frac{\sum\limits_{i=1}^{n} a_i p_i}{1 + \sum\limits_{i=1}^{n} a_i p_i} \quad \frac{b_i p_i}{1 + \sum\limits_{i=1}^{n} b_i p_i} \tag{8}$$

and in the m-th

$$\Theta_{i,m} = \frac{\sum\limits_{i=1}^{n} a_i p_i}{1 + \sum\limits_{i=1}^{n} a_i p_i} \left[\frac{\sum\limits_{i=1}^{n} b_i p_i}{1 + \sum\limits_{i=1}^{n} b_i p_i} \right]^{m-2} \frac{b_i p_i}{1 + \sum\limits_{i=1}^{n} b_i p_i} \tag{9}$$

The total adsorption i-th component is

$$\Theta_i = \sum_{j=1}^{m} \Theta_{i,j} = \frac{a_i p_i}{1 + \sum\limits_{i=1}^{n} a_i p_i} +$$

$$+ \frac{\sum\limits_{i=1}^{n} a_i p_i}{1 + \sum\limits_{i=1}^{n} a_i p_i} \quad \frac{b_i p_i}{1 + \sum\limits_{i=1}^{n} b_i p_i} \quad \sum_{j=0}^{m-2} \left[\frac{\sum\limits_{i=1}^{n} b_i p_i}{1 + \sum\limits_{i=1}^{n} b_i p_i} \right]^{j} \tag{10}$$

When m-tends to infinity

$$\Theta_i = \frac{a_i p_i + b_i p_i \sum\limits_{i=1}^{n} a_i p_i}{1 + \sum\limits_{i=1}^{n} a_i p_i} \tag{11}$$

Because

$$\frac{\Theta_{i,1}}{\sum\limits_{i=1}^{n} \Theta_{i,1}} = \frac{\Theta_{i,j}}{\sum\limits_{i=1}^{n} \Theta_{i,j}} \tag{12}$$

we get

$$\Theta_i = \frac{a_i p_i \left(1 + \sum_{i=1}^{n} b_i p_i\right)}{1 + \sum_{i=1}^{n} a_i p_i} \tag{13}$$

For the case of a pure component equations (11) and (13) reduce to equation (1). Equation (13) is the same as has been derived by *Gonzalez* and *Holland*[6] for bilayer gas mixtures adsorption. This adsorption isotherm was examined experimental by *Gonzalez* and *Holland*[7]. It follows from their studies, that adsorption of hydrocarbon mixtures on charcoal is satisfactorily described by equation (13).

References

[1] *Markham, E. C., Benton, A. F.*, J. Amer. Chem. Soc. **53**, 497 (1931).
[2] *Brunauer, S., Emmet, P. H., Teller, E.*, J. Amer. Chem. Soc. **60**, 309 (1938).
[3] *Hill, T. L.*, J. Chem. Phys. **14**, 265 (1946).
[4] *Arnold, J. R.*, J. Amer. Chem. Soc. **71**, 104 (1949).
[5] *Hüttig, G. F.*, Mh. Chem. **78**, 177 (1948).
[6] *Gonzalez, A. J., Holland, C. D.*, AIChE Journal **16**, 718 (1970).
[7] *Gonzalez, A. J., Holland, C. D.*, AIChE Journal **17**, 470 (1971).

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