

Flow Mechanism of Adsorbate Through Porous Media in Presence of Capillary Condensation

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The flow mechanism of adsorbable gas through the porous adsorbent in the presence of capillary condensation is interpreted, and a new transport model is derived by separately taking into account the hopping behavior of adsorbed molecules in the adsorbed phase and the viscous flow of capillary condensate. Surface flow coefficients including the contribution of capillary flow calculated with this model agree with published experimental data.

SCOPE

Besides gaseous diffusion and flow in pores, surface flow of physically adsorbed gases is important in evaluating the apparent mass transfer rate through porous media. Capillary condensation begins to occur in the fine pores with increase of the gas-phase pressure of the adsorbable gas, and not only surface flow but also flow of capillary condensate should be taken into account. The static behavior of capillary condensate is comparatively well-understood (Gregg and Sing, 1967; El-Sabaawi and Pei, 1977; Okazaki et al., 1978). The dynamical behavior has, however, been studied only by a few investigators (Carman and Raal, 1952; Gilliland et al., 1958), despite the research that would benefit many practical fields such as drying and adsorption processes.

For the case that capillary condensation is not taking place, the authors have proposed a random hopping model for surface flow by introducing the average holding times of the molecules adsorbed in the monolayer and multilayer as the time taken to

hop to a neighboring site (Okazaki et al., 1981). Surface flow coefficients can be explained well by this model in the range of monolayer to multilayer adsorption.

On the other hand, for the case that capillary condensation coexists, Gilliland et al. (1958) attempted to explain their experimental results by proposing that the transport mechanism is multilayer surface flow alone even though they recognized the existence of capillary condensation. There are, however, some experimental results which cannot be expressed by their correlating equation.

The purpose of this paper is to propose a transport model for the flow of adsorbable gas through porous media by taking into account the hopping behavior of molecules adsorbed in the adsorbed phase and the viscous flow of the capillary condensate. The calculated results by this model are compared with published data.

CONCLUSIONS AND SIGNIFICANCE

By taking into account the hopping behavior of monolayer and multilayer adsorbing molecules in the adsorbed phase and the viscous flow of capillary condensate separately, a transport model for surface flow in the presence of capillary condensation has been proposed. A new formula based on the model for the apparent surface flow coefficient, containing the contribution of flow of the capillary condensate, was derived to explain

the dependence of the amount adsorbed. This formula contains one experimental constant for the flow of the capillary condensate in addition to two experimental constants determined for conditions with no capillary condensation.

The published experimental data were correlated well by inserting the optimum values for the experimental constants in the proposed formula.

THEORETICAL CONSIDERATION

In the range of low partial pressure of the adsorbable gas, monolayer adsorption predominates, while multilayer adsorption gradually increases with increase of the pressure. Further, when the pressure is approaching the saturated pressure of the adsorbate, capillary condensation begins to occur in the pores of adsorbent. The adsorbed phase, which means the molecules

adsorbed in both monolayer and multilayer, can be considered to be gradually replaced by the capillary condensed phase. Therefore, the apparent adsorbed phase should be divided into the actual adsorbed phase and the capillary condensed phase to interpret the mechanism of surface flow.

Consider the case that a plug of porous adsorbent contacts the gases having different partial pressure of adsorbate on the both sides. In the adsorbed phase the transport of adsorbed molecules is caused by the gradient of the amount adsorbed, or more directly, the gradient of the number density of the hopping molecules. On the other hand, the transport of capillary

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condensate can be regarded as Poiseuille flow of viscous liquid filling the pores of the porous media, caused by the gradient of capillary force. Hence, the above two transport mechanisms should be considered separately.

Surface Flow in Adsorbed Phase

The surface flow phenomenon in the adsorbed phase is regarded as a random walk process of so-called "hopping molecules" on the surface. The authors have presented a new hopping model for surface flow in the previous paper (Okazaki et al., 1981). According to this model, the following correlating equation for the surface flow coefficient on the heterogeneous surface was derived.

$$D_s = \frac{D_{s0}(\theta_e/\theta) \int_{E_{a0}}^{E_{a0}} (e^{-aE/RT} - e^{-E/RT}) / \{(1 - e^{-E/RT})(1 - \theta_e(1 - \tau_1/\tau_0))\} g(E) dE}{\int_{E_{a0}}^{E_{a0}} g(E) dE} \quad (1)$$

where

$$\tau_1/\tau_0 = (e^{-aE_1/RT} - e^{-E_1/RT}) (1 - e^{-E_{a1}/RT}) / \{(e^{-E_{s1}/RT} - e^{-E_{a1}/RT}) (1 - e^{-E_1/RT})\} \quad (2)$$

The values of θ_e , E_{s1} , E_{a1} , E_{a0} and $g(E)$ in Eq. 1 can be estimated using the method proposed by the authors (Okazaki et al., 1981).

Eq. 1 contains two parameters a and D_{s0} that explains the dependence of the surface flow coefficient on the amount adsorbed and the temperature.

Even when capillary condensation coexists, the surface flow coefficient D_s in the adsorbed phase can be calculated by Eq. 1. Here it may be considered that the surface area which contributes to the surface flow decreases because of capillary condensation. Accordingly the surface flow rate in the adsorbed phase is given by Eq. 3.

$$N_d = -\rho_{app} D_s A (dq_{BET}/d\ell) \{(S_T - S_C)/S_T\} \quad (3)$$

where $(S_T - S_C)/S_T$ is the correcting term which accounts for the decrease of the surface area contributing to the surface flow. The surface flow has also been expressed as

$$N_d = -P_d A dp/d\ell \quad (4)$$

where P_d is the permeability in the adsorbed phase. Consequently, from Eqs. 3 and 4, P_d can be given by:

$$P_d = (D_s \rho_{app}) (dq_{BET}/dp) \{(S_T - S_C)/S_T\} \quad (5)$$

Flow of Capillary Condensate

The critical radii of occurrence of capillary condensation can be evaluated by the following Kelvin equation.

$$\ln(p/p_s) = -2\sigma V_L \cos \alpha / (rRT) \quad (6)$$

Also the capillary suction pressure is expressed as:

$$p_c = -2\sigma \cos \alpha / r \quad (7)$$

According to the Kelvin equation the capillary condensation successively proceeds from fine pores to the larger ones as the gas-phase pressure of adsorbate increases. Hence the high pressure side of the porous plug is filled with capillary condensate more readily than the low pressure side. Once the capillary condensed phase is formed, the capillary force due to surface tension (Eq. 7), is higher on the low pressure side than on the high pressure side.

Accordingly, if the gradient of the gas-phase total pressure exists, then both the gradients of the capillary force and the gas-phase total pressure act as driving forces in the transfer of the capillary condensate, and viscous flow of capillary conden-

sate ensues. Here, it is assumed that the resistance to flow among constituting capillaries is neglected (Krisher, 1963).

The Kozeny-Carman equation is given by:

$$\bar{u} = -(\epsilon^3 dp/d\ell) / (\mu_L K_c S_c^2 \rho_{app}^2) \quad (8)$$

where \bar{u} is the mean flow velocity of condensate. Eq. 8, which was derived for the flow of fluid through porous media, can be assumed to be valid for the case that capillary condensation occurs in all pores. Providing that the pores where the capillary condensation does not take place does not contribute to the flow of condensate, the porosity of the capillary condensed phase $\epsilon_r(V_c/V_T)$ and the surface area of that phase S_c might be used instead of ϵ and S in Eq. 8, respectively. From a force balance of

liquid flowing in the constituting capillaries.

$$(dp_c/d\ell)d\ell = \rho_L g \sin \phi d\ell - (dp_T/d\ell)d\ell + (dp/d\ell)d\ell \quad (9)$$

and substituting Eq. 9 into Eq. 8, the flux of capillary condensate N_c is expressed by:

$$N_c = (\rho_L/M) \bar{u} A = -\rho_L \epsilon_r^3 (V_c/V_T)^3 A (dp_c/d\ell + dp_T/d\ell - \rho_L g \sin \phi) / (\mu_L K_c S_c^2 \rho_{app}^2 M) \quad (10)$$

where the gravity term and the gradient term of the gas-phase total pressure are neglected because we treat microporous media ($r < 2.0 \times 10^{-6}$ cm) in the present study. Therefore, Eq. 11 is used to calculate N_c .

$$N_c = (\rho_L/M) \bar{u} A = -\rho_L \epsilon_r^3 (V_c/V_T)^3 A (dp_c/d\ell) / (\mu_L K_c S_c^2 \rho_{app}^2 M) \quad (11)$$

The gradient of the capillary force $(dp_c/d\ell)$ in Eq. 11 is related to the gas-phase pressure $(dp/d\ell)$ as follows. From Eqs. 6 and 7,

$$dp_c/d\ell = \{RT/(V_L p)\} dp/d\ell \quad (12)$$

If the difference of the gas-phase pressure across the porous plug is small, \bar{p} may be used instead of p in Eq. 12, where \bar{p} is the average gas-phase pressure. The permeability of the capillary condensate P_c is then derived from Eqs. 11 and 12.

$$P_c = -N_c / (A dp/d\ell) = \rho_L^2 \epsilon_r^3 (V_c/V_T)^3 RT / (\mu_L K_c S_c^2 \rho_{app}^2 M^2 \bar{p}) \quad (13)$$

In the case that all the pores in porous media are filled with capillary condensate ($V_T = V_c$), the permeability of capillary condensate P_c^0 is given as Eq. 14. Substituting $V_c/V_T = 1$, $S_c = S_T$ and $\bar{p} = p_s$ into Eq. 13 gives:

$$P_c^0 = \rho_L^2 \epsilon_r^3 RT / (\mu_L K_c S_T^2 \rho_{app}^2 M^2 p_s) \quad (14)$$

From Eqs. 13 and 14,

$$P_c = (S_T/S_c)^2 (V_c/V_T)^3 (p_s/\bar{p}) P_c^0 \quad (15)$$

If P_c^0 is obtained from an experiment, P_c can be estimated from Eq. 15.

Apparent Surface Flow Coefficient

The surface flow rate N_s is usually defined by the following equation, even for the case that capillary condensation coexists (Carman and Raal, 1951; Gilliland et al., 1958).

$$N_s = -P_{sapp} A (dp/d\ell) = -\rho_{app} D_{sapp} A (dq/d\ell) \quad (16)$$

where P_{sapp} and D_{sapp} contain the terms of the surface flow and the flow of capillary condensate, and are named as the apparent surface permeability and the apparent surface flow coefficient, respectively.

Providing that the transport paths in the capillary condensed phase and in the adsorbed phase are approximately independent

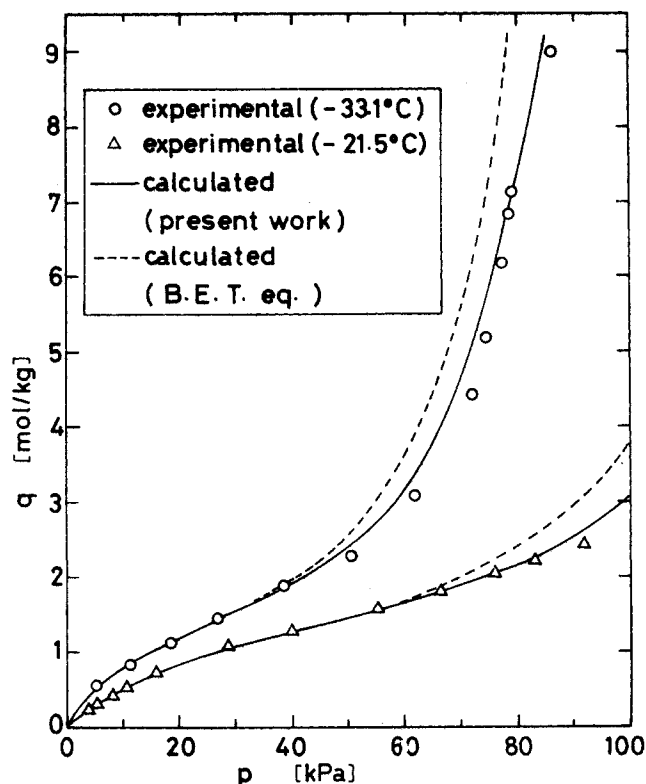


Figure 1. Adsorption isotherms of CF_2Cl_2 on Linde silica: experimental data by Carman and Rael (1951).

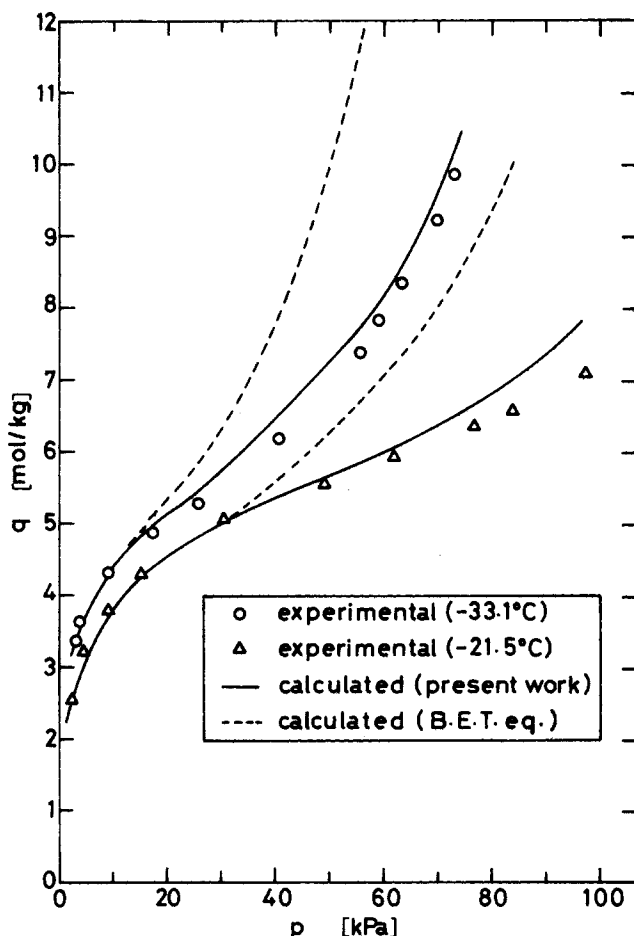


Figure 3. Adsorption isotherms of CF_2Cl_2 on Carbolac: experimental data by Carman and Rael (1951).

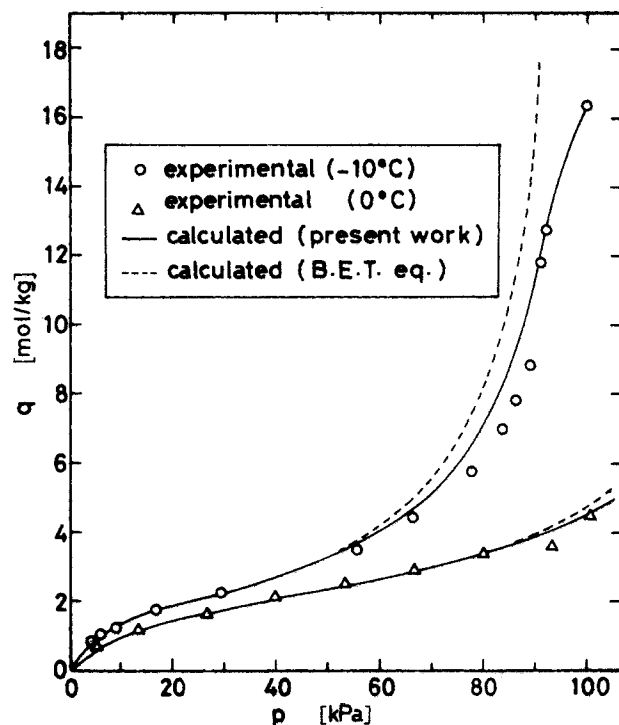


Figure 2. Adsorption isotherms of SO_2 on Linde silica: experimental data by Carman and Rael (1951).

each other, the apparent surface permeability P_{sapp} is given as $(P_c + P_d)$. Consequently the apparent surface flow coefficient D_{sapp} is expressed by Eq. 17.

$$D_{sapp} = (P_c + P_d) / \{(dq/dp)_{p_{app}}\} \quad (17)$$

where P_d and P_c are determined from Eqs. 5 and 15, respectively.

Volume and Surface Area of Capillary Condensed Phase

The volume V_c and the surface area S_c of the capillary condensed phase should be estimated to determine the apparent surface flow coefficient using Eqs. 5, 15 and 17. If an adsorption equilibrium in the phase without capillary condensation obeys the B.E.T. equation,

$$q_{BET} = q_m Cx / \{(1 - x)(1 - x + Cx)\} \quad (18)$$

The thickness of the adsorbed layer t can be evaluated by Eq. 19.

$$t = q_{BET} V_L / S_T \quad (19)$$

As the Kelvin radius r can be calculated from Eq. 6 by assuming that $\cos \alpha = 1$, capillary condensation occurs in the pores whose radii are smaller than $(r + t)$. Accordingly, V_c and S_c can be estimated from the pore-size distribution of the adsorbent. Providing that the B.E.T. type adsorption takes place uniformly on the surface of adsorbent, the amount adsorbed q_d in the phase where capillary condensation does not occur is given as Eq. 20.

$$q_d = (S_T - S_c) q_{BET} / S_T \quad (20)$$

The amount adsorbed q can be evaluated as the sum of that adsorbed in the adsorbed phase q_d and that in the capillary condensed phase q_c (Okazaki et al., 1978).

$$q = q_c + q_d \quad (21)$$

where q_c can be calculated from V_c .

THEORETICAL RESULTS AND DISCUSSIONS

Adsorption Equilibrium

Figures 1 to 4 present comparisons of the experimental adsorption isotherms (Carman and Rael, 1951; Gilliland et al., 1958) and calculated isotherms from Eqs. 18 to 21. The good

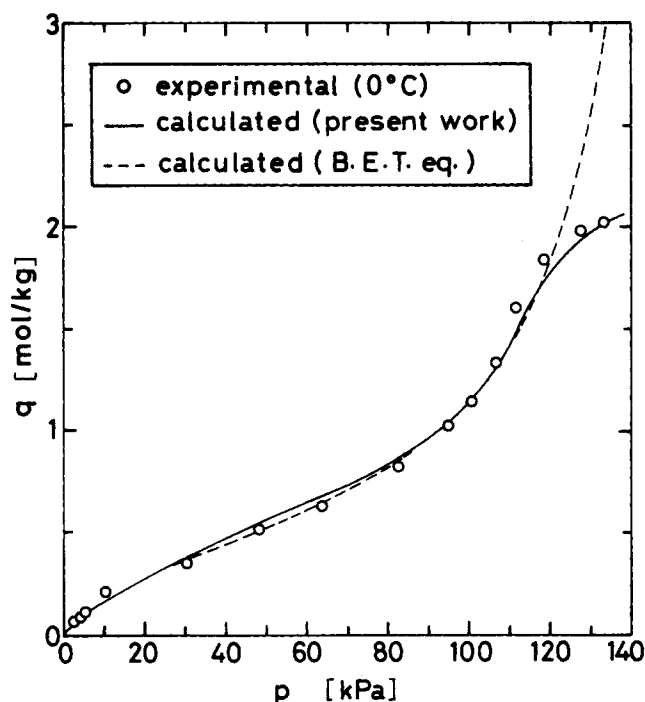


Figure 4. Adsorption isotherm of iC_4H_{10} on Vycor: experimental data by Gilliland et al. (1958).

agreement indicates the validity of the method for the determination of V_C and S_C . The B.E.T. equation, on the other hand, satisfies the experimental results for small amount adsorbed, but this equation overestimates the amount adsorbed with increase of the amount adsorbed.

The pore-size distribution used for the above calculations of V_C and S_C was the distribution reported by Carman and Raul (1951) for Linde-silica, and that calculated by their method for Carbolac. Further, the distribution for Vycor glass was estimated from an adsorption isotherm of iC_4H_{10} at $0^\circ C$ using the method proposed by Dollimore and Heal (1964). Here the thickness of adsorbed layer t was evaluated by Eq. 19.

Apparent Surface Flow Coefficient

The B.E.T. equation can be applied for the adsorbed phase and the surface flow coefficient can be calculated by Eq. 1 for a heterogeneous surface. The optimum values of a and D_{s0} in Eq. 1 have been reported in the previous paper entitled "In-

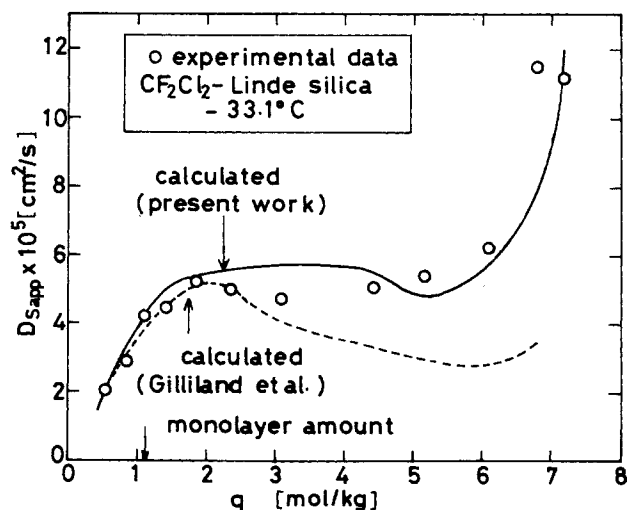


Figure 6. Apparent surface flow coefficients of CF_2Cl_2 on Linde silica: experimental data by Carman and Raul (1951).

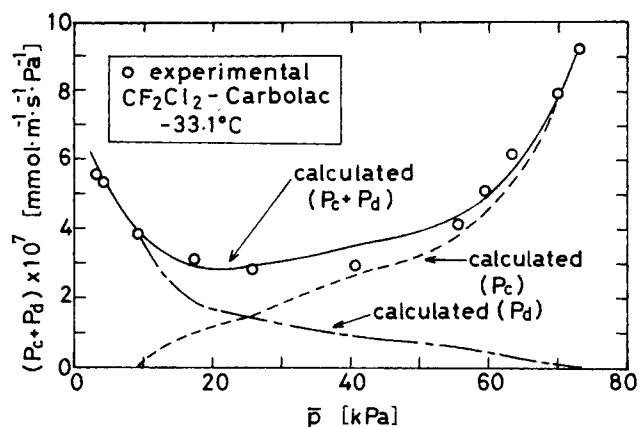


Figure 5. Permeabilities of CF_2Cl_2 through Carbolac: experimental data by Carman and Raul (1951).

terpretation of Surface Flow Phenomenon of Adsorbed Gases by Hopping Model." These values were determined for conditions of a small amount adsorbed where capillary condensation does not take place.

The permeability of the adsorbed phase P_d can be calculated from Eqs. 1 and 5, where S_C and q_{BET} can be evaluated by Eqs. 6, 18 and 19 and the pore-size distribution. For the capillary condensed phase the permeability of the condensate P_c can be estimated by Eq. 15, where V_C can be calculated by Eqs. 6, 18 and 19 and the pore-size distribution. The calculated P_d , P_c and $(P_c + P_d)$ for the flow of CF_2Cl_2 through Carbolac are shown in Figure 5. There it can be seen that P_d decreases with the average pressure \bar{p} or the amount adsorbed q , while P_c increases. This figure shows that the calculated values of $(P_d + P_c)$ agree well with the experimental values. Accordingly, the apparent surface flow coefficient D_{sapp} can be correlated by Eq. 17.

Figures 6 to 12 show the calculated apparent surface flow coefficients, and the values of P_c^0 used for the calculation are listed in Table 1. The calculated results using Eq. 22 proposed by Gilliland et al. (1958) are also shown in these figures.

$$D_{sapp} = C' q (d \ln p) / (d \ln q) \quad (22)$$

The model proposed in the present work satisfactorily represents the experimental apparent surface flow coefficients. On the other hand, Eq. 22 considerably underestimates the experimental results as shown in Figures 6, 8, 10 and 11, even though it represents the experimental values shown in Figures 7, 9 and 12.

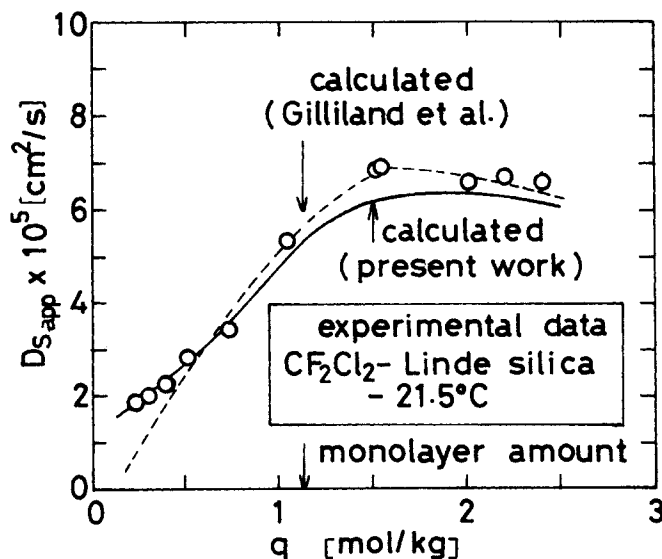


Figure 7. Apparent surface flow coefficients of CF_2Cl_2 on Linde silica: experimental data by Carman and Raul (1951).

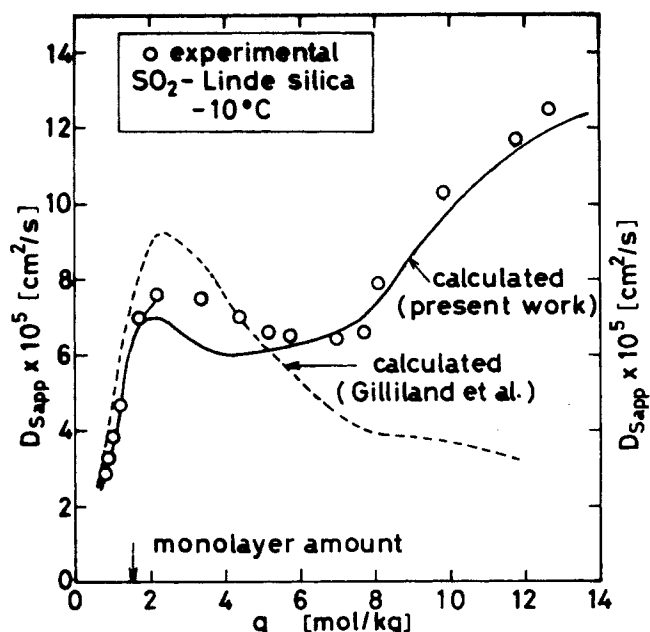


Figure 8. Apparent surface flow coefficients of SO_2 on Linde silica: experimental data by Carman and Raul (1951).

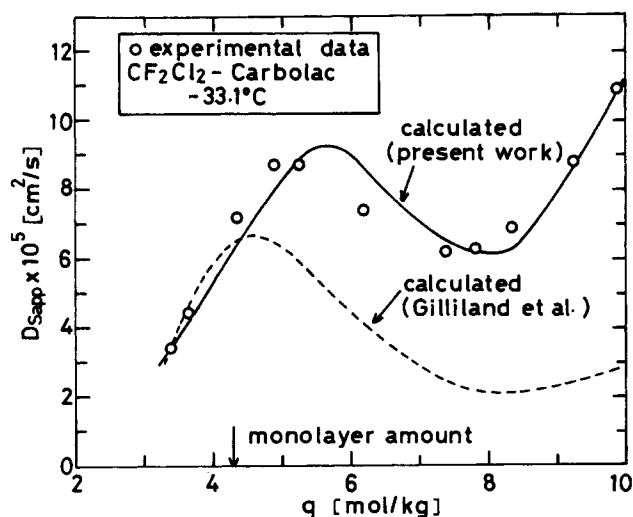


Figure 10. Apparent surface flow coefficients of CF_2Cl_2 on Carbolac: experimental data by Carman and Raul (1951).

The change of D_{sapp} with the amount adsorbed displays the typical inverse S-shaped curve, such as shown in Figures 6, 8, 10 and 12. This change can be explained by the present model as follows. The surface flow coefficient increases with the amount adsorbed in the range of monolayer adsorption based on Eq. 1. When multilayer adsorption begins in the adsorbed phase and capillary condensation is formed in finer pores, the number of adsorbed molecules contributing to surface flow and the surface area ($S_T - S_C$) begins to decrease. Hence, P_d decreases according to Eq. 5. On the other hand, the increase of P_c only makes up for the decrease of P_d , because the flow resistance of the capillary condensate is large in the finer pores. So, $(P_d + P_c)$ does not show a large increase, while the slope of adsorption isotherm (dq/dp) suddenly increases with the gas-phase pressure. Accordingly, the apparent surface flow coefficient D_{sapp} changes to show the maximum value due to Eq. 17. As the capillary condensation proceeds further, P_c increases and D_{sapp} rises again, and gives the minimum value of D_{sapp} . From the above consideration, the apparent surface flow coefficient follows the inverse S-shaped dependence on the amount adsorbed.

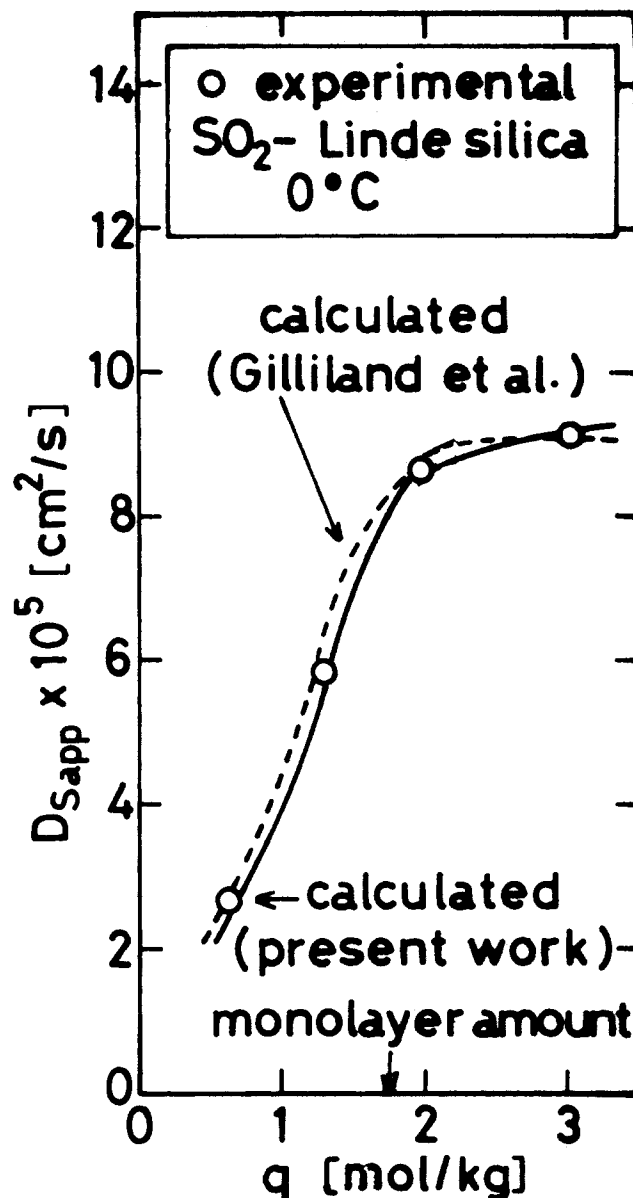


Figure 9. Apparent surface flow coefficients of SO_2 on Linde silica: experimental data by Carman and Raul (1951).

Discussion of P_c°

The value of P_c° can be determined from the following two methods. It is determined from the experimental permeability in the case where all pores are filled with condensate or from the parameter fitting using experimental data. Also the value can be predicted by Eq. 14. In the present work the value of P_c° was estimated from experimental data, because it is difficult to evaluate the Kozeny constant K_C in Eq. 14. However, we consider that the discussion of K_C is necessary to predict the apparent surface flow coefficient.

The Kozeny constant K_C is usually taken to be 5. This value is almost valid for unconsolidated beds such as granular sand beds, while the value is many times greater than 5 for abnormal pore textures. Wyllie and Rose (1950) preferred to modify the Kozeny treatment and proposed the following equation.

$$K_C = 2.5k_e^2 \quad (23)$$

where k_e is the tortuosity factor. The constant K_C calculated from Eq. 14 and P_c° is listed in Table 1. The value of k_e evaluated by Eq. 23 is also presented in Table 1. It can be seen that the values

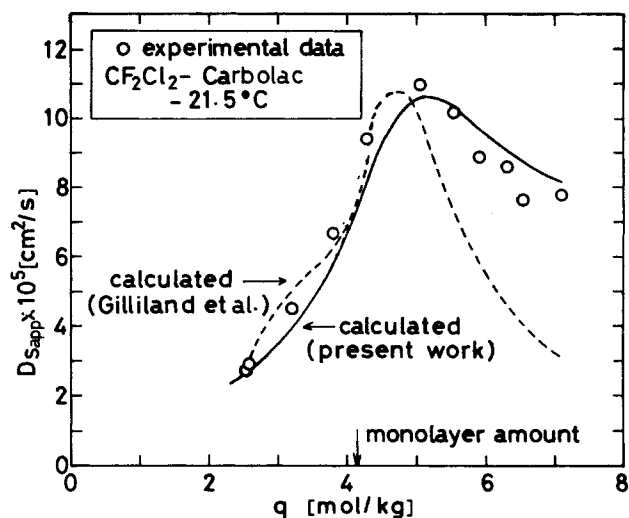


Figure 11. Apparent surface flow coefficients of CF_2Cl_2 on Carbolac: experimental data by Carman and Raal (1951).

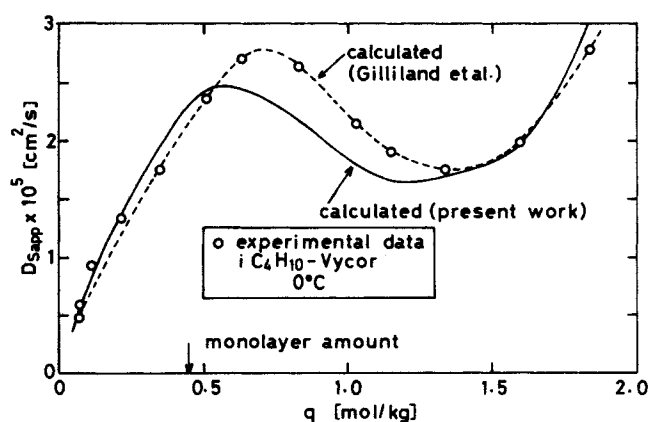


Figure 12. Apparent surface flow coefficients of $i\text{C}_4\text{H}_{10}$ on Vycor: experimental data by Gilliland et al. (1958).

TABLE 1. VALUES OF P_c° , K_c , k_c AND k_k

System	Temp. °C	P_c°	K_c	k_c	k_k Eqs. 24 and 25
CF_2Cl_2 -Linde	-33.1	6.87×10^{-6}	6.47	1.60	1.41
Silica ¹	-21.5	4.01×10^{-6}	6.47	1.60	1.41
SO_2 -Linde	-10.0	2.16×10^{-5}	6.47	1.60	1.41
Silica ¹	0.0	1.42×10^{-5}	6.47	1.60	1.41
CF_2Cl_2 -Carbolac ¹	-33.1	1.45×10^{-6}	4.25	1.30	1.63
Carbolac ¹	-21.5	8.92×10^{-7}	4.25	1.30	1.63
$i\text{C}_4\text{H}_{10}$ -Vycor ²	0.0	3.82×10^{-7}	16.3	2.55	2.21

Experimental data: 1) Carman and Raal (1951); 2) Gilliland et al. (1958).

of k_c are nearly equal to the ones for most of consolidated media reported by Wyllie et al. (1950 and 1952).

The tortuosity factor k_k for the Knudsen flow can be estimated from the following equation. According to the parallel pore model (Okazaki et al., 1981),

$$P_g = 2\epsilon_T \bar{r} \sqrt{8RT/(\pi M)} / (3k_k^2 RT) \quad (24)$$

where P_g is the Knudsen permeability and \bar{r} is the average pore radius ($=2V_T/S_T$). Asaeda et al. (1974) proposed the following equation for packed beds of particles of nonuniform diameters.

$$P_g = 8\epsilon_T^2 \sqrt{1/(2\pi MRT)} / (k_k^2 \Phi S_T \rho_{app}) \quad (25)$$

where $\Phi = 2.18$.

The values of k_k calculated by Eq. 24 or 25 are also presented in Table 1. As the value of k_k does not agree with that of k_c at least for the system examined in the present paper, the prediction method of K_c from the Knudsen flow has a considerable error. Therefore, more detailed investigations about the tortuosity factor and the Kozeny constant are needed to predict the flow of capillary condensate.

NOTATION

A	= cross-sectional area of sample, cm^2
a	= constant
C	= constant defined in Eq. 18
C'	= constant defined in Eq. 22, $\text{cm}^2 \cdot \text{kg} \cdot \text{s}^{-1} \cdot \text{mol}^{-1}$
D_s	= surface flow coefficient, cm^2/s
D_{sapp}	= apparent surface flow coefficient, cm^2/s
D_{s0}	= constant defined in Eq. 1, cm^2/s
E_{a0}	= differential heat of adsorption, kJ/mol
E_{a1}	= heat of vaporization, kJ/mol
E_{s1}	= activation energy for migration in all layers above the first layer, kJ/mol
g	= acceleration of gravity, $\text{m} \cdot \text{s}^{-2}$
$g(E)$	= number of molecules adsorbed which have the heat of adsorption between E and $(E + dE)$
K_c	= Kozeny constant
k_c	= tortuosity factor for flow of capillary condensate
k_k	= tortuosity factor for Knudsen flow
ℓ	= dimension along plug axis, cm
M	= molecular weight, kg/kmol
N_c	= flow rate of capillary condensate, mol/s
N_d	= rate of surface flow in adsorbed phase, mol/s
P_c	= permeability of capillary condensate, $\text{mmol} \cdot \text{m}^{-1} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}$
P_c°	= permeability in the case that all pores are filled up with capillary condensate, $\text{mmol} \cdot \text{m}^{-1} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}$
P_d	= permeability of surface flow in adsorbed phase, $\text{mmol} \cdot \text{m}^{-1} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}$
P_g	= Knudsen permeability, $\text{mmol} \cdot \text{m}^{-1} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}$
P_s	= permeability of surface flow, $\text{mmol} \cdot \text{m}^{-1} \cdot \text{s}^{-1} \cdot \text{Pa}^{-1}$
p	= pressure, kPa
\bar{p}	= average pressure, kPa
p_c	= capillary force, kPa
p_f	= pressure due to friction, kPa
p_s	= saturated vapor pressure, kPa
q	= amount adsorbed, mol/kg
q_{BET}	= amount adsorbed calculated by B.E.T. equation mol/kg
q_m	= monolayer amount adsorbed, mol/kg
R	= gas constant, $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
r	= pore radius, cm
\bar{r}	= average pore radius, cm
S	= surface area, m^2/kg
S_c	= specific surface area of capillary condensed phase, m^2/kg
S_T	= specific surface area, m^2/kg
T	= temperature, K
t	= thickness of adsorbed layer, cm
\bar{u}	= average velocity of capillary condensate, cm/s
V_c	= volume of capillary condensed phase, cm^3/kg
V_L	= molar volume ($=M/\rho_L$), cm^3/mol
V_T	= total pore volume, cm^3/kg
x	= relative pressure ($=p/p_s$)

Greek Letters

α	= contact angle
ϵ	= porosity
ϵ_T	= porosity of porous media
θ	= surface coverage ($=q/q_m$)
θ_e	= effective surface coverage for surface flow
μ_L	= viscosity in liquid state, $\text{Pa} \cdot \text{s}$

ρ_{app} = apparent density, kg/cm³
 ρ_L = density in liquid state, kg/cm³
 σ = surface tension, N/m
 ϕ = horizontal angle

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An Efficient, General Method for Computation of Countercurrent Separation Processes with Axial Dispersion

A calculational method is proposed for the simulation of steady-state, multi-solute, countercurrent extraction with axial dispersion. The method provides for complex chemical-equilibrium and phase-equilibrium relationships, and accounts for the individual resistances of the liquid phases in the calculation of mass-transfer rates. The solution procedure follows that developed by Newman (1967, 1968) for systems of simultaneous, second-order difference equations.

Three example problems are solved to demonstrate the efficiency and flexibility of the method. These include (1) an example from McSwain and Durbin (1966), (2) calculation of axial-dispersion and mass-transfer parameters from experimental data for the extraction of acetic acid from water by a tertiary amine in an RDC extractor, and (3) simultaneous extraction of solutes that interact in an acid-base complexing reaction at the liquid-liquid interface. The examples all assume that extraction is governed by interphase mass-transfer rates and cell-wise backmixing; however, the method is also applicable to equilibrium-stage separators, separators described by the diffusional model of axial dispersion, and other countercurrent separation processes.

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It is well established that axial dispersion can have a large, adverse impact on the performance of separation devices. While many previous workers have proposed calculational methods that allow prediction of the effects of axial dispersion (Mecklenburgh and Hartland, 1975; etc.), these methods are generally limited to simple situations, as when one can assume a constant degree of axial dispersion throughout the device,

linear or quadratic phase-equilibrium relationships, constant overall mass-transfer coefficients, and the interphase transfer of either a single solute, or multiple dilute, non-interacting solutes. The goal of the present work was to develop a calculational method that could be applied to more general problems. This was motivated by the need to analyze experimental mass-transfer data obtained in a small-scale liquid-liquid extraction column for systems exhibiting complex phase-equilibrium behavior. The performance of the column appeared to be dominated by axial dispersion.

The laboratory column was a rotating disk contactor (RDC). In the proposed calculational method, the RDC was represented by a series of well-mixed cells connected by forward and

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