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Simulation of Solute Diffusion through Porous Media

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ABSTRACT

Simulation of solute diffusion through porous media (membrane) was carried out by a random walk procedure. The porous media used were three kinds of two-dimensional square networks of channels with almost the same average pore diameters and porosities, but with different pore size distributions. In the simulation the partition equilibrium of solute between the bulk feed phase and the membrane phase was established, and the apparent permeability in the steady state was evaluated. First, only the steric interaction between the solute and the pore wall was considered. In spite of the similar average pore diameters and porosities of the networks, the apparent permeability and selectivity were dependent on the kinds of networks. The network with more small pores showed the smaller permeability and the higher selectivity. When the diameter of solute which can be actually transported is fairly smaller than the average pore diameter, the network with broad pore distribution and with more small pores is found to be useful for obtaining higher selectivity. Next, the electrostatic and dispersion (van der Waals) interactions between the solute and the pore wall were introduced in this simulation. By such long-range interactions the selectivity increased while the apparent permeability decreased. This result showed that the introduction of the repulsive electrostatic interaction between membrane and solute is one useful method for enhancing the selectivity. The effects of the kinds of networks on transport properties in the presence of long-range interactions were similar to those in the absence of such interactions.

Key Words. Solute diffusion; Porous model; Random walk; Random channel widths; Partition coefficient

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INTRODUCTION

Transport in porous media plays an important role in membrane separations, in various chromatographics, and in catalysis operations. Porous membranes have been especially well utilized in such operations as microfiltration, ultrafiltration, and dialysis. These membranes have contributed to water and gas purification, metal recovery, drug release, and so on.

Many studies have been carried out on the clarification of pore structures of porous membranes, especially with respect to microfiltration and ultrafiltration membranes (1–4). The relations between membrane structures and membrane performances have been clarified qualitatively. When pore size distributions are clarified or given, it is very important to predict ultrafiltration or dialysis separation results quantitatively. These predictions are significant for producing novel functional membranes as well as for designing the membrane process. However, as MacDonald pointed out (5), there have been few studies from such points of view.

One method to predict membrane performances for a given membrane structure is a computer simulation of solute transport. Sahimi et al. simulated the dispersion in porous media and found it was described by the convective-diffusion equation (6). They showed that the dispersion was sensitive to pore radius distribution, pore coordination and blockage, and the orientation of pores with mean flow direction. Imdakm and Sahimi (7) and MacDonald (8) investigated particle migration or diffusion in the given networks by the random walk procedure. The percolation properties of the networks were discussed in these studies. Sahimi and Jue (9) and Sahimi (10) studied hindered transport of large molecules in networks of pores. They not only considered diffusion, but also convection. Moreover, the effect of van der Waals interaction between particles and walls on the transport of large particles in networks of capillary tubes were discussed in the literature (11, 12). Since these studies were not always intended for porous membranes, the separation of various particles or solutes was not focused upon in these studies.

MacDonald modeled macromolecule diffusion through various porous media, and the selectivity of diffusion with respect to molecular size was monitored (5). It was found that wall–molecular interaction and molecular size had an important effect on diffusion. The selectivity, which was defined as the ratios of diffusivity, was discussed with respect to the pore distribution and network connectivity. However, partition of solute between bulk solution and membrane phase, which is usually established in actual membrane operation such as dialysis, was not taken into account.

In this study the particle (solute) transport was investigated by the random walk procedure on three different irregular two-dimensional networks. These networks have almost the same average pore diameters and pore porosities. The purpose of this work is to clarify the effect of the network structure; that is, pore distribution on the solute transport by simulation. It is almost impossible to create real membranes with the same average pore diameters and pore porosities, and with different pore distributions. Therefore, the goal of this work could be achieved only by computer simulation. For the relation between a particle and one certain pore, a theory on the hindered diffusion of a particle into a pore has been well developed (13). Numerical results have been presented not only about the case which includes only steric and hydrodynamic interactions between a particle and the pore wall, but also about the case involving electrostatic and/or dispersion (van der Waals) interactions (14–16). Based on the theories, we evaluated solute partitioning between the bulk solution and the membrane phase, and the residence time of the particle in the pores in the two cases; that is, in the case with only steric interaction and also in the case with electrostatic and dispersion interactions as well as steric interaction.

In the usual pore–network simulation, the solutes are initially placed at the edge of the network (membrane) and the unsteady motion of the solutes is monitored. In this original simulation, however, partition equilibrium was assumed at one end of the network (feed phase) and the particles transported at the other end (receiving phase) by each step were considered to be permeability in the steady state. These simulations correspond to those for solute transport in membrane dialysis.

SIMULATION METHOD

Porous Media

The porous medium is represented by a two-dimensional square network. The conceptual figure for the network is schematically shown in Fig. 1. The y-direction is the transport direction. The bonds of the network, which represent the channels of the porous medium, are assumed to be cylindrical capillary tubes with the same length. The network consists of 1250 sites (50 sites for the x-direction and 25 sites for the y-direction). The diameters D of the channel are distributed according to the density functions $f(D)$. The locations of the channels of each width in the network were determined by random numbers. Three different networks were formed by three density functions, that is, Gauss density function with large variance ($\sigma = 0.133$), Gauss density function with small variance ($\sigma = 0.1$), and linear density function. These networks are referred as wide Gauss, narrow Gauss, and linear networks in what follows. All

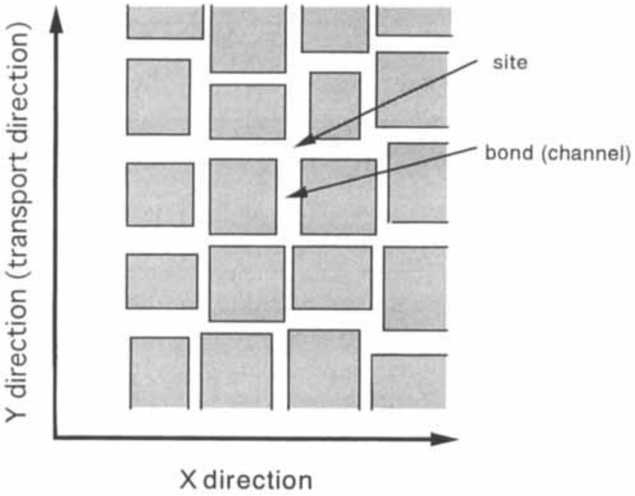

FIG. 1 Conceptual figure for two-dimensional square network.

density functions are normalized as $\int_0^\infty f(D)dD = 1$. These functions, expressed as Eqs. (1)–(3), are shown in Fig. 2.

$$f(D) = 1/(\sqrt{2\pi}\cdot 0.133)\exp\{-(D-0.5)^2/(2\cdot 0.133^2)\}$$

(for wide Gauss network) (1)

$$f(D) = /(\sqrt{2\pi}\cdot 0.1)\exp\{-(D-0.5)^2/(2\cdot 0.1^2)\}$$

(for narrow Gauss network) (2)

$$f(D) = -8.820D + 7.384$$

(for linear work) (3)

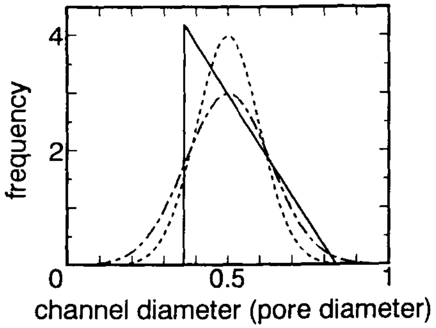

FIG. 2 Three kinds of density functions: (- - -) Gauss density function with large variance, (---) Gauss density function with small variance, (——) linear density function.

These channel width (pore) distributions are referred to those of the commercial membranes. A pore distribution close to Gaussian distribution was reported for the Sartorius cellulose acetate microfilter membrane (SM11106) (3), and that close to linear distribution was reported for the polysulfone membrane (IRIS-3026, Rhone-Poulenc) (4).

The average pore diameter $\bar{D}$ can be calculated by using the density functions as follows.

$$\bar{D} = \int_0^\infty f(D) D\, dD \tag{4}$$

The porosity of the network P is given by

$$\begin{aligned} P &= \left(N \int_0^\infty f(D) \pi (D/2)^2 dD \right) / A \\ &= \pi N/(4A) \int_0^\infty f(D) D^2 dD \end{aligned} \tag{5}$$

where N is the pore (channel) number in the phase perpendicular to the y-direction and A is the area of that phase, which is not considered in this work because a two-dimensional square network was used. The value of $\pi N/(4A)$ is constant irrespective of the kind of network. The values of $\bar{D}$ and $\int_0^\infty f(D)D^2dD$ for three networks are listed in Table 1. The values of $\bar{D}$ and $\int_0^\infty f(D)D^2dD$ are almost the same for each network. This means that each network has almost the same average pore diameter and porosity. Therefore, the difference in the particle (solute) transport characteristics through the networks is attributable to only the difference in pore distributions.

Transport Procedure

The partitioning between sites at $y = 0$ (bulk feed phase) and those at $y = 1$ (membrane phase) was considered. All the sites (50) in the x-direction at $y = 0$ were assumed to be occupied by solute molecules (particles). The number of solutes occupying the sites at $y = 1$ was determined by considering both the solute size and pore sizes (bond sizes) at $y = 0$

TABLE 1

Values of $\bar{D}$ and $\int_0^\infty f(D)D^2dD$ for Various Networks

	$\bar{D}$	$\int_0^\infty f(D)D^2dD$
Wide Gauss network	0.500	0.271
Narrow Gauss network	0.500	0.263
Linear network	0.518	0.280

according to the partition coefficients described below. If solutes on sites at $y = 1$ move, other solutes were supplied on those sites, and the ratio of the solute number at $y = 1$ to that at $y = 0$, which is the partition coefficient, was maintained at a constant value at any time. This condition corresponds to equilibrium partitioning between the bulk feed phase and the membrane phase.

From the sites at $y = 1$, solutes undergo a random walk through the network described above, and their progress to the other boundary site ($y = 26$) is followed. Periodic boundary conditions are employed in the x-direction. According to MacDonald's method (5), the random walk is biased in the y-direction, which corresponds to the condition that a driving force for the transport exists in the y-direction. This bias is imposed by always considering the possibility of motion in the positive y-direction first. When this motion is impossible due to the smaller pore size than the solute size, or if the channel of the y-direction is already occupied by the solute, the motion of the $\pm x$-direction is considered to have equal possibility. If the pore sizes of the bonds of the $\pm x$-direction are smaller than the solute size, the solute remains at the site.

The solutes are moved from one site to another through the channel based on the residence time in the channel. As described below, the ratio of diffusivity of hindered transport D_H to bulk diffusivity D_∞, D_H/D_∞, is given by Eqs. (13) and (14). The reciprocal of the ratio is employed as the residence time. Therefore, when the pore is fairly large and the diffusion in the pore is the same as that in the bulk phase, the solute is transported through the channel in one step. When the pore size is comparable to the solute size, several steps, whose number is equal to D_∞/D_H for the solute to move through the channel, are needed. For each step the solutes transported to the far side of the network ($y = 26$) are counted as the permeation number. Although several solutes with different sizes were used, we considered the diffusion of a certain solute individually and not the case of the solute mixture.

In order to check the effect of network size, simulation was carried out for a network two times larger with respect to the y-direction. Although the results showed lower apparent permeabilities compared with those in the usual network, the effects of the various network types shown in Fig. 2 on the apparent permeabilities and selectivites were similar.

Partition Coefficient

For the hindered transport of rigid solutes in cylindrical pores, the partition coefficient Φ, the ratio of the average interpore concentration $\langle C \rangle$ to that in bulk solution C is expressed as follows (13).

$$\Phi = \langle C\rangle/C = 2\int_0^{1-\lambda} \exp(-E(\beta))\beta d\beta \tag{6}$$

where λ is the ratio of solute diameter to pore diameter, E is the potential describing long-range interactions (electrostatic and dispersion forces) between the solute and the pore wall (which is assumed to depend only on the radial position), and β is the dimensionless radial position in the pore ($= r/r_0$, r = radial position, r_0 = pore radius).

An important special case is that of purely steric interactions between the solute and the pore wall ($E = 0$). In this case the following equation is obtained.

$$\Phi = (1 - \lambda)^2 \tag{7}$$

As approximation expressions for either the attractive (van der Waals) or the repulsive (double layer) energy describing a sphere in a cylindrical pore, we used those for a sphere interacting with a infinite plate. The sphere–plate interaction energy for dispersion force E_a is given by

$$E_a = H/(6kT)[\ln(1 + 2a/h) - 2(a/h)(1 + a/h)/(1 + 2a/h)] \tag{8}$$

where H is the Hamaker constant, k is the Boltzmann constant, T is the temperature, a is the solute radius, and h is the shortest distance between the solute surface and pore wall ($r_0 - r - a$) (14). The sphere–plate interaction energy for overlapping double layers, E_r, is expressed as follows (14).

$$E_r = [16\epsilon akT/e^2] \tanh\{e\xi_p/(4kT)\} \tanh\{e\xi_w/(4kT)\} \exp(-\kappa h) \tag{9}$$

where ϵ is the solution dielectric constant, e is the charge on an electron, ξ_p and ξ_w are the surface potentials of the solute surface and pore wall, respectively, and κ is the Debye parameter. At 298 K for a 1:1 electrolyte in water, the value of κ in Å unit is calculated to be

$$\kappa = 3.04/\sqrt{C_s} \tag{10}$$

where C_s is an electrolyte concentration in molarity (14). Malone and Anderson presented the following approximation for the interaction energy of latex–mica (14)

$$\begin{aligned} E \approx\ & 0.4[\ln(1 + 2a/h) - 2(a/h)(1 + a/h)/(1 + 2a/h)] \\ & + 1.0 \times 10^3 \exp(-\kappa h) \end{aligned} \tag{11}$$

As one typical example, we evaluated the long-range interaction energy by using Eq. (11). The units of pore diameter and solute diameter have not been considered by us because we made the simulation more general.

Since the transport characteristics are almost determined by the ratio of solute diameter to pore diameter λ in the case considering only steric interaction, the units are not very significant and various units are possible to use. However, when Eq. (11) is used, a unit of h (that is, a unit of the pore diameter) has to be determined. Because dialysis (gel) membranes with pore sizes of 50 to 100 Å have often been reported (17, 18), we used a value of 0.5 for the pore size in Fig. 2, correspond to 75 Å, and calculated the interaction energy by Eq. (11). The partition coefficient Φ in the presence of long-range interactions was obtained by substituting the interaction energy E in Eq. (6) and integrating the equation.

Residence Time

The ratio of the diffusivity of hindered transport D_H to the bulk diffusivity D_∞ is expressed as follows for the hindered transport of rigid solutes (13).

$$\frac{D_H}{D_\infty} = \frac{\int_0^{1-\lambda} K^{-1}(\lambda, \beta) \exp(-E(\beta))\beta d\beta}{\int_0^{1-\lambda} \exp(-E(\beta))\beta d\beta} \tag{12}$$

where $K(\lambda, \beta)$ is an enhanced drag coefficient. The usual "centerline approximation" that $K(\lambda, \beta)$ is approximated by $K(\lambda, 0)$ (13) was adopted by us. The centerline approximation leads to Eq. (13) regardless of the value of E.

$$D_H/D_\infty = K^{-1}(\lambda, 0) \tag{13}$$

Bungay and Brenner presented the following equation for $K^{-1}(\lambda, 0)$ as accurate even for larger value of λ (19).

$$K^{-1}(\lambda, 0) = 6\pi/[9/4\pi^2\sqrt{2}(1-\lambda)^{-5/2}\{1 - 73/60(1 - \lambda) + 77293/50400(1-\lambda)^2\} - 22.5083 - 5.6117\lambda - 0.3363\lambda^2 - 1.216\lambda^3 + 1.647\lambda^4] \tag{14}$$

Although Eq. (16) was derived for $E = 0$, $K^{-1}(\lambda, 0)$ is independent of E when the centerline approximation is adopted. Therefore, we evaluated the value of D_H/D_∞ by Eq. (14) both in the absence and in the presence of long-range interactions. As described above, the reciprocal of D_H/D_∞ was used as the residence time in the channel. Since integers need to be used as the residence time, the values of D_∞/D_H were rounded off to integers.

RESULTS AND DISCUSSION

Case Considering Only Steric Interaction between Solute and Pore Wall

Figure 3 shows the effects of pore diameters and solute diameters on the partition coefficient ϕ and the residence time. Only the steric interaction between the solute and the pore wall was considered in this case. The partition coefficient was calculated by Eq. (7), and the residence time was obtained as the reciprocal of D_H/D_∞ as calculated by Eq. (14). The partition coefficient decreased monotonously with decreasing the pore diameter and increasing the solute diameter, due to the exclusion effect. Contrarily, the residence time increased with a decrease in the pore diameter and with an increase in the solute diameter. As the solute diameter approaches the pore diameter, the residence time increases abruptly. The extremely large residence time means that it is actually impossible for the solute to move in the channel.

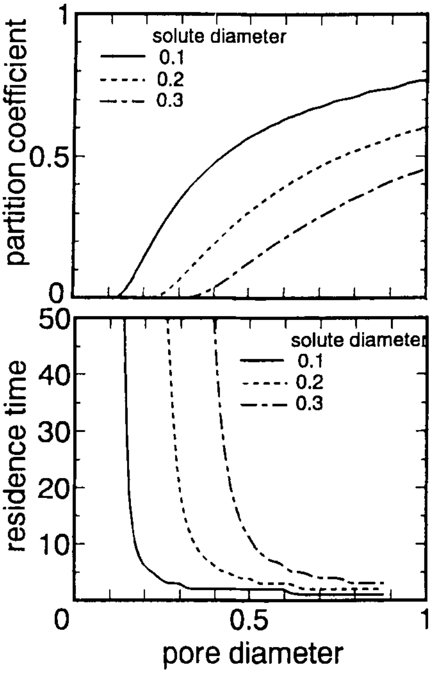

FIG. 3 Effect of pore diameter and solute diameter on partition coefficient and residence time.

Figure 4 shows the relation between the permeation number and the step number for a wide Gauss network. The permeation number is the number of solutes transported to the far side of the network for each step. In the region of large step numbers, nearly constant permeation numbers were obtained. These nearly constant values can be regarded as the apparent permeabilities in the steady state. These values in the steady state decrease with an increase in the solute diameter. In what follows, these apparent permeabilities in the steady state are considered.

The effects of the kinds of networks on the partition coefficient and the apparent permeability are shown in Fig. 5. The partition coefficients were hardly influenced by the kinds of networks. On the other hand, the permeabilities were clearly dependent on the kinds of networks. Although the networks have almost the same average pore diameter and porosity, a difference in the pore distributions brings about a difference in the permeabilities. The apparent permeability for a linear network is largest, and that for a wide Gauss network is lowest.

According to the solution-diffusion mechanism, the permeability is given by the product of the partition coefficient and the diffusivity. The apparent diffusivities obtained by dividing the permeability by the partition coefficient are shown in Fig. 6. The data shown in Fig. 5 for the permeabilities and the partition coefficients were used in the calculation. The diffusivities were dependent on the kinds of networks, and the order of magnitude of the diffusivities was the same as that of the apparent permeabilities. Even if the average pore diameter and porosity are nearly

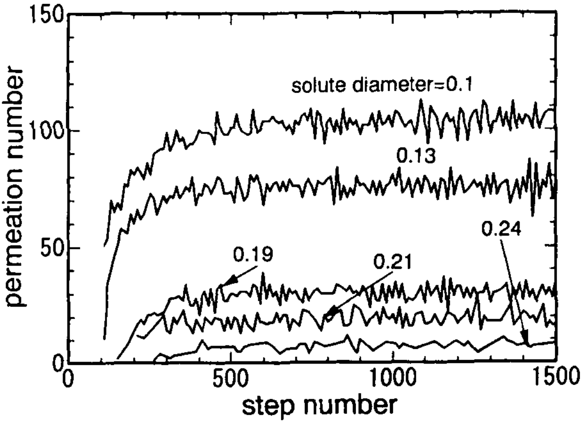

FIG. 4 Relation between permeation number and step number for wide Gauss network.

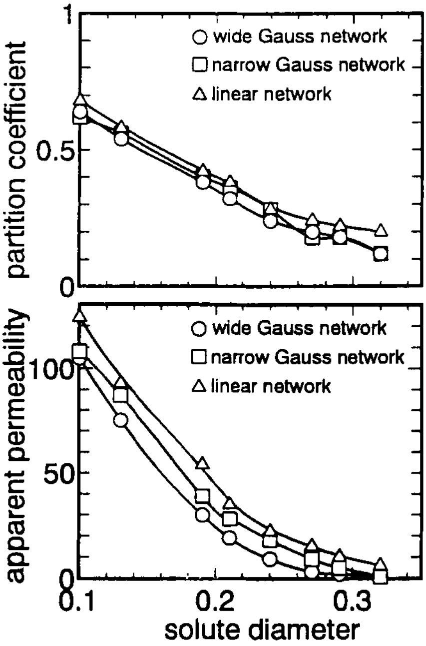

FIG. 5 Effect of kinds of networks on partition coefficient and apparent permeability.

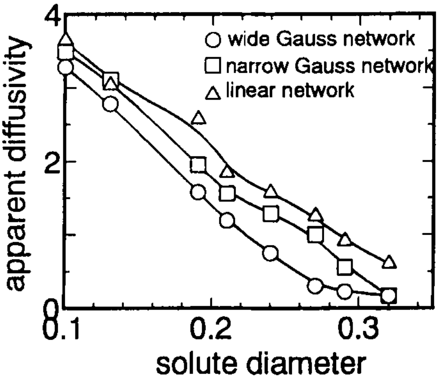

FIG. 6 Effect of kinds of networks on apparent diffusivity.

the same for each network, the total diffusion property decreases for a network with more small pores in which the solute cannot be transported or remains for a long time. Therefore, the wide Gauss network showed the lowest diffusivity because the network has more small pores, as shown in Fig. 2. For each network the order of magnitude of fractions of small pores corresponds inversely to the order of diffusivity. In the series of channels from one side of the network to the other side, the existence of only one small pore brings about an extreme decrease in the diffusivity. Therefore, diffusivity is sensitive to the fraction of small pores. On the other hand, the partition coefficient mainly depends on the fraction of large pores and is not as sensitive to the fraction of small pores. This is the reason why the dependence of the partition coefficients on the kinds of networks is weak, as shown in Fig. 5. In this system the difference in the diffusivities reflects the difference in the apparent permeabilities for each network.

Figure 7 shows the effects of the kinds of networks on selectivity. Selectivity is defined as the ratio of the apparent permability for a solute with a diameter of 0.1 to that for a larger solute. Selectivity shows a tendency opposite to that of the apparent permeability. That is, the wide Gauss network showed the largest selectivity and the linear network showed the lowest. When the pore size is sufficiently large, solutes can be transported in the channel by one step regardless of the solute sizes. This means that a large pore cannot distinguish the differences in solute diameters. On the other hand, a small pore can recognize the difference in solute sizes more clearly. This is the reason why selectivity becomes higher for a network with more small pores in spite of the smaller apparent permeability. A

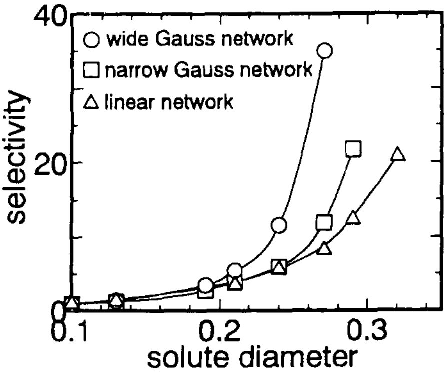

FIG. 7 Effect of kinds of networks on selectivity.

network with a sharp pore distribution is usually considered to give high selectivity. This is true only in the case where the average pore diameter is approximately in agreement with the diameter of a solute which can be transported. It should be noted that when the diameter of a solute is fairly smaller than the average pore diameter used in this simulation system, a network with a broad pore distribution and with more small pores can give higher selectivity.

Case Considering Electrostatic and Dispersion Interactions in Addition to Steric Interaction

When there are electrostatic and dispersion (van der Waals) interactions between the solute and the pore wall, the interaction energy E is given in Eq. (11) for the case of latex–mica interaction. The partition coefficients obtained by substituting the interaction energy E in Eq. (6) are shown in Fig. 8 for various electrolyte concentrations. Because the repulsive (double layer) forces are predominant in this case, the partition coefficients decrease when the long-range interactions are introduced. As shown in Eq. (10), the Debye parameter κ, which is a length scale over which the electrostatic interaction occurs, increases as the electrolyte concentration decreases, so that the solute is repelled from the pore wall over a greater range of distances. Thus, the partition coefficients decrease with a decrease in the electrolyte concentration, as shown in Fig. 8.

As described above, the ratio D_H/D_∞ is independent of the interaction energy E as far as the centerline approximation is employed. Therefore,

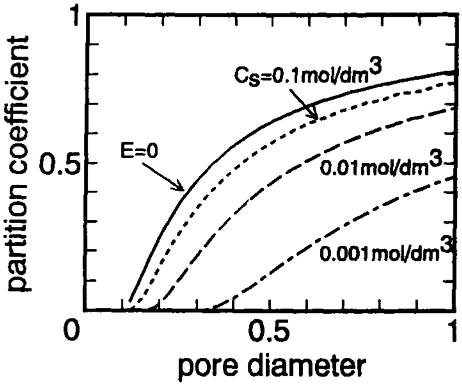

FIG. 8 Partition coefficient in the presence of long-range interactions. Solute diameter = 0.1.

the same value was used as the residence time both in the absence and in the presence of long-range interactions.

Figure 9 shows the apparent permeability and selectivity in the presence of long-range interactions. By introducing those interactions, the apparent permeability decreases, and the decrease becomes more significant with a decrease in the electrolyte concentrations. This is attributable to a decrease in the partition coefficient as shown in Fig. 8. On the other hand, the introduction of long-range interactions brings about an increase in selectivity. The repulsive (double layer) force is not uniform for the solutes with different diameters, and it has a tendency to increase as the solute diameter increases and approaches pore size. Therefore, when long-range interaction is considered, the apparent permeability decreases more sharply with an increase in the solute diameter due to increasing repulsive force in addition to the normal exclusion effect. This is the reason why the selectivity, which is defined as the ratio of the apparent permeability

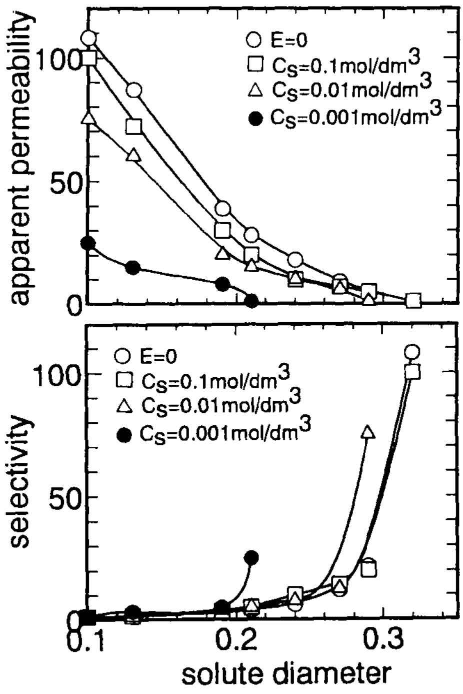

FIG. 9 Apparent permeability and selectivity in the presence of long-range interactions: narrow Gauss network.

for a solute with a diameter of 0.1 to that of a larger solute, increases when long-range interactions are introduced. This simulation clearly shows that introduction of repulsive electrostatic interaction to a membrane separation system is effective from the standpoint of enhancing selectivity.

The effects of the kinds of networks on the apparent permeability and selectivity are shown in Fig. 10. These are simulation results for an electrolyte concentration of 0.1 mol/dm^3. The tendency of the apparent permeability and selectivity is the same as that for the case considering only steric interaction. That is to say, the linear network shows the largest permeability and the lowest selectivity, and the wide Gauss network gives the smallest permeability and the highest selectivity. Although the introduction of long-range interactions results in a decrease in the partition coefficient, the degree of decreases in the partition coefficients is not very different for various networks. This leads to similar effects on the trans-

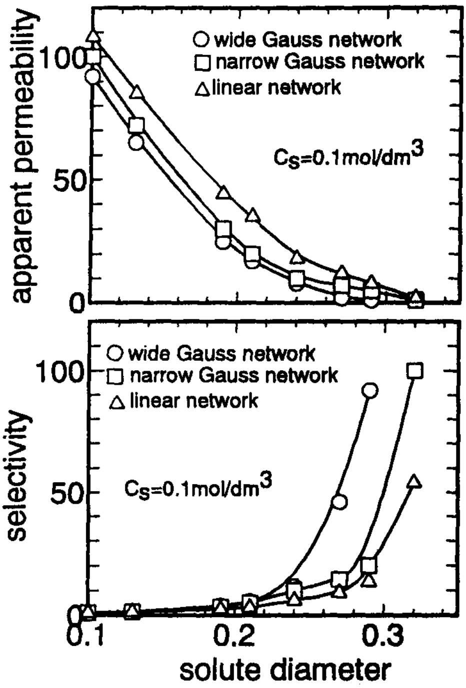

FIG. 10 Effect of kinds of networks on apparent permeability and selectivity in the presence of long-range interactions.

port properties of various kinds of networks both in the absence and in the presence of long-range interactions.

CONCLUSIONS

Simulation of particle (solute) diffusion through porous media (membrane) was carried out for various networks with almost the same average pore diameters and porosities, but with different pore size distributions. The partition equilibrium of solute between the bulk feed phase and the membrane phase was established at the feed side, and the apparent permeability in the steady state was evaluated. The conclusions obtained were as follows.

1. When only the steric interaction between the solute and the pore wall was considered, the partition coefficients were not very different for various networks. However, the apparent permeability and selectivity were clearly dependent on the kinds of networks; that is, on the pore size distributions. The network with more small pores showed smaller permeability and higher selectivity.
2. Furthermore, long-term interactions such as the electrostatic and dispersion (van der Waals) interactions between the solute and the pore wall were considered. By the introduction of these interactions, the apparent permeability decreased, and the decrease became more significant with a decrease in the electrolyte concentration. On the other hand, the introduction of these interactions brought about an increase in selectivity. Thus, it was confirmed in this simulation that the repulsive electrostatic interaction between the solute and the pore wall is effective for enhancing selectivity. The effects of the kinds of networks on transport properties were similar to those in the case considering only steric interaction.

SYMBOLS

A	area of phase perpendicular to y-direction
a	solute radius
C	bulk concentration
C_s	electrolyte concentration (mol/dm^3)
$\langle C \rangle$	average interpore concentration
D	channel (pore) diameter
$\bar{D}$	average channel (pore) diameter
D_H	diffusivity of hindered transport
D_∞	bulk diffusivity

$E(\beta)$	potential describing long-range interactions between solute and pore wall
E_a	interaction energy for dispersion force
E_r	interaction energy for overlapping double layers
e	charge on electron (C)
$f(D)$	density function
H	Hamaker constant (J)
h	shortest distance between solute surface and pore wall ($= r_0 - r - a$)
K	enhanced drag coefficient
k	Boltzmann constant (J/K)
N	pore number in phase perpendicular to y-direction
P	porosity of network
r	radial position in pore
r_0	pore radius
T	temperature (K)

Greek

α	variance of Gauss density function
β	dimensionless radial position in pore ($= r/r_0$)
ϵ	solution dielectric constant
ϕ	partition coefficient
κ	Debye parameter (m^{-1})
λ	ratio of solute diameter to pore diameter
ξ_p	surface potential of solute surface (J/C)
ξ_w	surface potential of pore wall (J/C)

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