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Abstract: Monte Carlo simulation method is employed to investigate separation behavior of gas mixture composed of carbon dioxide and nitrogen through a model carbon membrane under the different conditions. The simulation gives insight into the separation mechanism to a certain extent, which is based on the loading and diffusion of carbon dioxide and nitrogen in the carbon membrane with different pore size. The simulation results indicate that the carbon dioxide can be adsorbed on the surface of membrane wall more strongly, whereas the diffusion rate of nitrogen is more prominent. When the separation condition alters, the influence of the two main factors mentioned above on transport of gas molecules in membranes becomes different. Therefore, the equilibrium selectivity of nitrogen and carbon dioxide changes correspondingly.

Keywords: Carbon membrane, gas separation, molecular simulation, adsorption and diffusion

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INTRODUCTION

More attention has been paid to remove carbon dioxide from atmosphere because it is affecting our environment (1, 2). So it is very necessary to develop effective technologies for gas separation. Among them, gas separation by means of a membrane process has been currently of fundamental and practical interest. In general, commercial membranes are made mainly from organic material. However, their poor thermal and chemical resistances limit their use to a certain extent (3–4). Alternatively, inorganic membranes have been applied widely in the field of gas separation due to their outstanding advantages such as stability to high temperature and high-pressure, high selectivity, high rates of transport, and so on (5–8). As a consequence, the inorganic membrane characteristics have been investigated widely and deeply through different experimental approaches. However, as far as we know, the relevant theories are not clearly established for permeation phenomena in porous membranes. There are still no systematic rules to identity membrane properties and performances. Therefore, it is essential to understand separation mechanism of gas mixtures based on molecular interaction and membrane structure (9–11).

Molecular simulation techniques, composed of the Monte Carlo (MC) and molecular dynamics (MD) method, have become powerful tools to study static and dynamic properties of molecular system (12). Due to the incorporation of Newton's equations of motion, MD simulation can provide relatively detailed information about the system following the evolution of system with time. However, this method is highly computer intensive. In contrast, MC simulation is less computer intensive than MD though it only supplies a less rigorous account of diffusion since the dynamics are not described by those Newton's equations of motion. Therefore, MC simulations have been widely applied to investigate surface diffusion in zeolites and other systems (6, 13, 14).

In this report, MC method is employed to calculate the equilibrium selectivity of carbon dioxide and nitrogen in nano-porous carbon membranes under the different separation conditions. Furthermore, the adsorption and diffusion of CO_2/N_2 binary gas mixture in the model carbon membrane are investigated in detail. Based on these, the separation mechanism of the carbon membrane for CO_2/N_2 system is explored tentatively from the microcosmic scope.

SIMULATION

Simulation Methods

A standard canonical Monte Carlo simulation (15) is employed in the present research. In this method, the temperature, the volume, and the sum of all species are kept constant. The standard procedure of the Metropolis sampling with the periodic condition in y and z directions is applied. Initially, nitrogen and carbon dioxide molecules are randomly placed in the simulation box except the membrane region. The molecular translation is considered in the simulation. In the random movement, the maximum displacement is 0.03 nm. The motion is accepted by a certain probability of 25% ~ 35% in the simulation.

In all of the computations, the carbon dioxide and nitrogen molecules are modeled as structureless particles which interact with each other and with the carbon atoms of the membrane via the truncated and shifted force form of the Lennard-Jones 12-6 potential (16):

$$\varphi_{ij}^{SF} r_{ij} = \varphi_{ij} r_{ij} \ \ \varphi_{ij} r_{rcut} \frac{d\varphi_{ij} r_{ij}}{dr_{ij}}\bigg|_{rcut} r_{ij} \ r_{cut}, \quad r_{ij} \leq r_{cut} = 0 \quad r_{ij} > r_{cut}$$

With

$$\phi_{ij}(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

where r_{cut} is the cut-off distance and σ_{ij} and ε_{ij} are the co-diameter and potential well depth for particles *i* and *j*, respectively. The potential parameters employed in this work are summarized in Table 1 (16–18). For all the cross-term LJ parameters, the Lorentz-Berthelot combination rules have been employed to compute the terms for unlike species, i.e. $\varepsilon_{ij} = \sqrt{((\varepsilon_{ii}\varepsilon_{jj}))}$ and $\sigma_{ij} = (\sigma_{ii} + \sigma_{jj})/(2)$. In the simulations, the potential was truncated at 3.0 σ_{ij}.

Molecular Model

In the simulation, the equilibrium selectivity, adsorption, and diffusion of CO_2/N_2 mixture in a carbon membrane with slit pores are investigated. The pore is represented by a slit, bounded by blocks of graphite. Despite its simple geometry, this pore model has been used successfully to characterize carbon adsorbents and predict adsorption in these materials (19–22). The fundamental cell for the molecular simulation consists of 10 basal graphite layers above and below a single isolated pore. Therefore, the membrane itself is

Table 1. LJ parameters used in the simulation

Group	σ (nm)	ε/k (K)
CO_2	0.3910	225.3
N_2	0.3798	71.4
C	0.34	28.2

regarded as a set of isolated pores each separated by 20 basal graphite layers in the z direction and of infinite width in the y direction. The two sides of the membrane pore is symmetrical along the x co-ordinate axis. The membrane thickness remains constant. The membrane is composed of 4200 carbon atoms, which are placed regularly according to the structure of graphite layers. The distance between graphite layers is 0.335 nm. The width of the membrane pores varies between 0.4 and 1.7 nm.

In the simulation, the effects of several factors such as the slit width, the pressure, and the composition on the equilibrium selectivity of the gas mixture are considered. Figure 1 shows a schematic diagram of the simulation cell used in the present work. Just as the literature described (17), two volumes labeled as H and L, respectively, are placed on each side of the membrane. Volume H and volume L stand for the high-pressure and low-pressure sides of the membrane at beginning of the simulation, respectively. In addition, the co-ordinate system is defined as follows: the flow is in x-direction and graphite planes are distributed along the z-direction.

A concentration gradient for the diffusing species is imposed across the porous membrane in order to provide the driving force for transport. At the beginning of each simulation, predetermined numbers of molecules of each species are placed in the H-region to reflect the pressure and composition of bulk gas phase on the high-pressure side of the membrane.

The equilibrium selectivity, S_{eq}, is defined by

$$S_{eq(CO_2/N_2)} = \frac{(x_{CO_2}/(y_{CO_2})}{(x_{N_2})/(y_{N_2})},$$

where x is the separated mole fraction and y is the bulk mole fraction. The diffusion of carbon dioxide and nitrogen are calculated by using the mean squared displacement (MSD) of the gas molecules. A Monte Carlo step (MCS) was defined as the process in which all molecules in the simulation

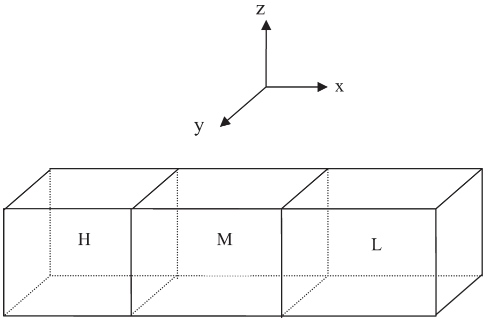

Figure 1. Schematic representation of the pore used in the simulations. The H and L and M areas correspond to the high and low pressure areas, and membrane, respectively. Transport is in the x direction.

cell finished one trial of random movement, and one MCS was assumed to be equal to a time duration of 10^{-14} s.

The diffusion coefficients of gas molecules in the membrane are estimated from the slope of their MSDs for long time. In general, the relation between MSD and time follows Einstein's equation,

$$D = \lim_{t \to \infty} \frac{\langle (r - r_0)^2 \rangle}{6t}$$

Where D is the diffusion coefficient, $\langle (r - r_0) \rangle^2$ is the MSD of the gas molecules.

RESULTS AND DISCUSSION

Equilibrium Selectivity of CO_2/N_2 Mixture under Different Separation Conditions

Simulations are carried out for mixed-gas permeation through carbon membranes with different pore sizes, system pressure, and bulk composition. In all simulations, the temperature is set at 300 k and the pressure was calculated according to the Redlich-Kwong equation (23).

Figure 2 shows the variation of the equilibrium selectivity of carbon dioxide over nitrogen as function of pore width when the pressure is 2.94 bar. During the simulation process, the membrane thickness remains constant, whereas the pore width ranges from 0.4 to 1.7 nm. And, the

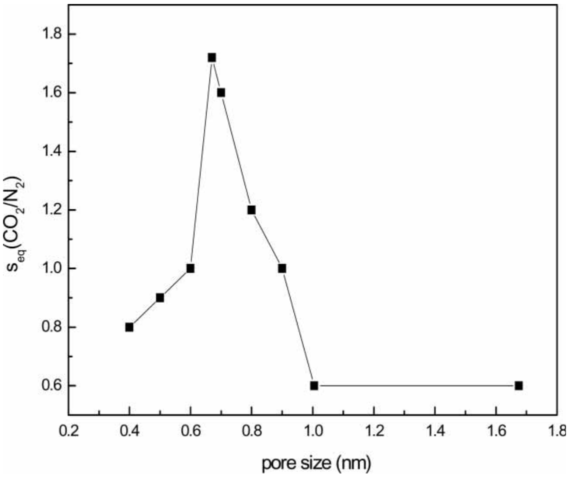

Figure 2. Variation of equilibrium selectivity with pore width at 300 k for CO_2/N_2 ratio of 1, with constant membrane thickness.

mixed-gas is an equi-molar mixture of carbon dioxide and nitrogen. Obviously, from this figure, it is interesting to note that the carbon membrane with a different pore width will display different separation behavior for the CO_2/N_2 mixture. When the pore width is smaller than 0.6 nm or bigger than 0.9 nm, nitrogen molecules are separated from the gas mixture to a certain extent. However, carbon dioxide molecules will be separated preferentially from the gas mixture when the pore width ranged from 0.6 to 0.9 nm. And, it can be seen clearly that the equilibrium selectivity of carbon dioxide achieves a maximum of selectivity when the pore width is about 0.66 nm. Furthermore, the simulation results also indicate that the equilibrium selectivity is very sensitive to variation of the pore size, especially in the range (i.e. from 0.6 to 0.9 nm). That is, the separation factor is as much as 1.7 when the pore size is 0.66 nm, whereas the separation factor of the carbon membrane with 0.6 nm pore size is almost equal to 1.

The effect of pressure on the separation behavior of an equi-molar CO_2/N_2 mixture system is also investigated. Figure 3 depicts the changes of the equilibrium selectivity of carbon dioxide and nitrogen with the increase of system pressure from 1.47 to 4.41 bar when the pore width is set as 1.0 nm. From this figure, it can be seen that the equilibrium selectivity of carbon dioxide declines with the increase of system pressure. That is to say, the increase of the system pressure is beneficial to the separation of nitrogen from gas mixture to a certain extent. However, it is worth noting that, compared with the change of separation behavior resulting from the

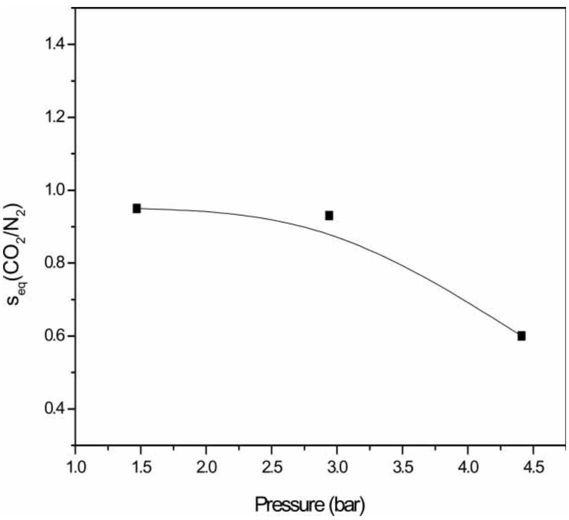

Figure 3. Equilibrium selectivity of CO_2/N_2 as a function of pressure at 300 k.

variation of pore size, the alteration of system pressure only has a relatively less influence on the separation factor of the gas mixture.

Figure 4 shows the effect of the composition on the equilibrium selectivity of CO_2/N_2 system when the pore width is 1.0 nm and the pressure is 2.94 bar. It can be seen that a higher equilibrium selectivity of carbon dioxide can be achieved with the increase of fractions of carbon dioxide in the feed, namely an increase of the separation factor from about 1 to 1.35 with the increase of carbon dioxide fraction from about 0.6 to 0.8. This may be related to the competitive adsorption between carbon dioxide and nitrogen on the pore surface. That is, the fewer the amount of nitrogen molecules in the mixture gases is, the more the loading of carbon dioxide in the membrane pore may become. Therefore, this is apt to result in the increase of the equilibrium selectivity of carbon dioxide over nitrogen. This explains partly why the relatively low carbon dioxide fraction (for an example, $y_{CO_2} = 0.5$) may be beneficial to the separation of nitrogen, which has been illustrated in Fig. 4. However, it can be seen that, just like the role played by the system pressure, the influence resulting from the alteration of the system composition also seems to be inferior to that of the pore size. Through investigating the effects of the pore size, the system pressure, and the composition of the separation behavior of gas mixture by the carbon membrane, it is reasonable to think that pore width is a key factor for gas separation.

Some references (24–25) have shown that the permeation rate of gases in the inorganic membrane is primarily determined by two rate-determining factors:

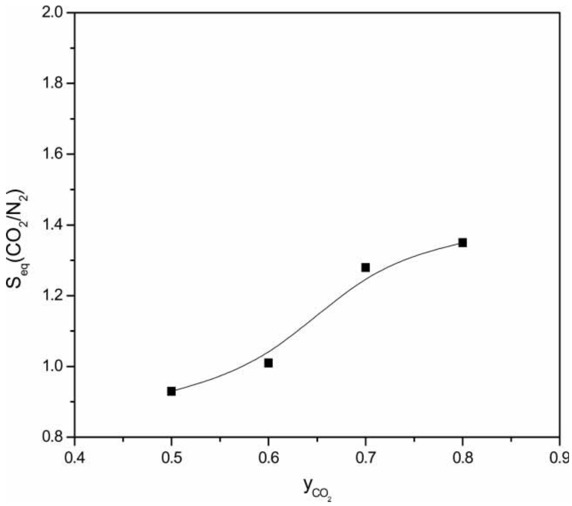

Figure 4. Equilibrium selectivity of CO_2/N_2 as a function of composition at 300 k.

1. Loading of the gases inside the membrane; and
2. Diffusion of gases through the membrane pore.

In order to probe the potential mechanism of pore width effect on the equilibrium selectivity from the microcosmic scope, we calculate the density profiles of carbon dioxide and nitrogen and their mean squared displacement in carbon membranes with different pore sizes such as 0.4 nm, 0.66 nm, and 1.0 nm.

Density Profiles

Figures 5–7 show the equilibrium adsorption profiles of carbon dioxide and nitrogen in the membrane with different pore sizes. These results demonstrate that the adsorbed gas mixture within the membrane pore is truly two-dimensional. It can be seen clearly from these figures that the peaks for carbon dioxide (solids lines) are always higher than those for nitrogen (broken lines). In other words, the loading of carbon dioxide in the membrane pores is always larger than that of nitrogen. This can be explained by their difference of the adsorption power in carbon membranes. Furthermore, combined with the corresponding separation behavior of carbon membranes with different pore sizes depicted in Fig. 2, it can be concluded that the separation selectivity of the specified gas is not proportion to its loading in the membranes. Moreover, these figures also clearly show that the transport of carbon dioxide and nitrogen are close to the pore wall. In other words, this means that surface diffusion makes an important contribution to the mass transport of the gas mixtures through the carbon membrane.

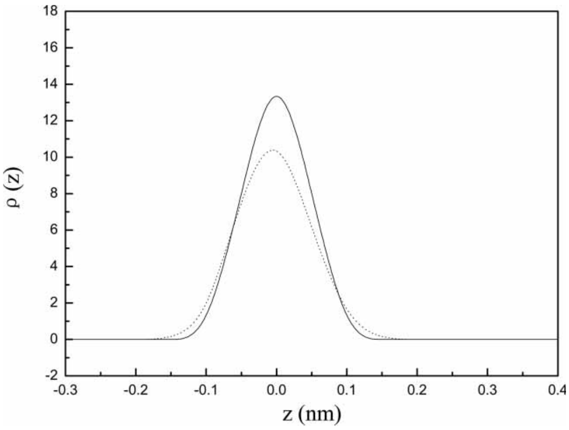

Figure 5. Density profiles for mixed-gas in the membrane pore with 0.4 nm; solid lines denote CO_2 and broken lines N_2.

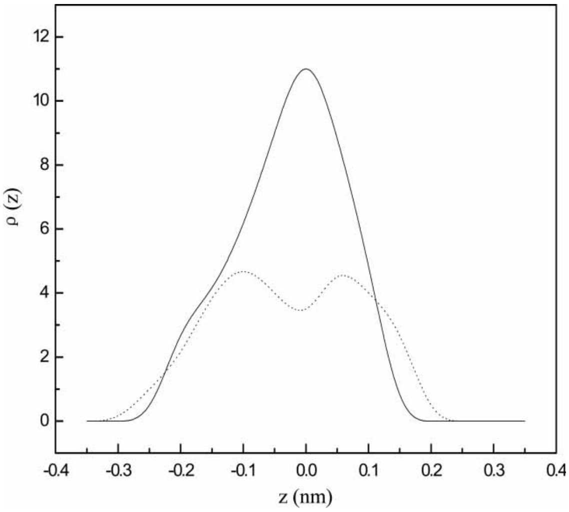

Figure 6. Density profiles for mixed-gas in the membrane pore with 0.66 nm; solid lines denote CO_2 and broken lines N_2.

In addition, it is found from Fig. 5 and Fig. 7 that both carbon dioxide and nitrogen molecules are adsorbed on the pore wall in a single layer when the pore width is 0.4 nm, whereas their adsorption take on a two-layer structure when the pore size is 1.0 nm. Moreover, it is worth noting that the peaks for either carbon dioxide or nitrogen appear at a similar location. Obviously, this indicates that carbon dioxide and nitrogen must be adsorbed on the same layer in the membrane pore with the pore sizes mentioned above. This

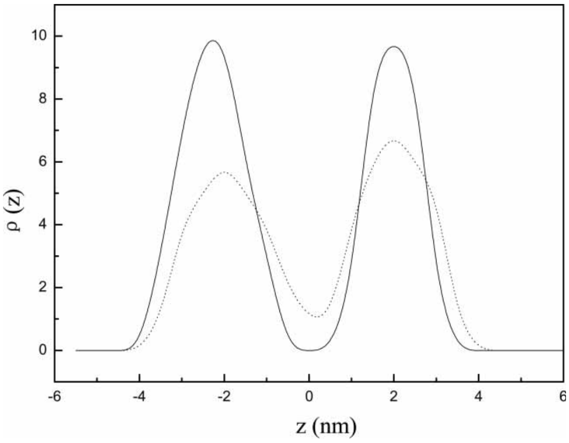

Figure 7. Density profiles for mixed-gas in the membrane pore with 1.0 nm; solid lines denote CO_2 and broken lines N_2.

may attribute to their similar potential parameters σ which are demonstrated in Table 1. Therefore, it is reasonable to conclude that they will be adsorbed on the membrane pore surface competitively when they penetrate to the low pressure region through surface diffusion.

In contrast, Fig. 6 demonstrates that the nitrogen molecules are mainly adsorbed on the pore surface in two layers while most of the carbon dioxide molecules are adsorbed in a single layer, namely in the center of the membrane pore when the pore size is 0.66 nm. Obviously, this indicates that, for the specified pore size, carbon dioxide and nitrogen molecules are not adsorbed on the same layer in the membrane pore though they possess similar potential parameters. Coincidentally, just as the simulation results depicted in Fig. 2, the carbon membrane with this pore size can obtain the maximum of equilibrium selectivity of carbon dioxide and nitrogen molecules. This may be attributed to the fact that the affinity strength resulting from the attractive forces between the gas molecule and the wall is stronger in the case of simultaneous interactions with both walls. And, this simultaneous interaction becomes important when the pore diameter is less than approx. 3 times that of the gas molecule diameter, like in these systems. As a consequence, the carbon dioxide molecules are capable of diffusing effectively through the center of the pore with less interference of nitrogen molecules to the low pressure region. Besides, the fact that good permeability for carbon dioxide molecules is obtained in this case also proves further that the permeation of the gas mixture across the carbon membrane may follow surface diffusion mechanism.

Based on the above research, it is reasonable to think that the rates of surface diffusion of carbon dioxide and nitrogen molecules affect the equilibrium selectivity of a CO_2/N_2 system directly. Furthermore, in order to understand the separation mechanism of a CO_2/N_2 system in carbon membrane, it is necessary to investigate the mean squared displacement of carbon dioxide and nitrogen in carbon membrane with different pore width.

The Mean Squared Displacement of Carbon Dioxide and Nitrogen in Carbon Membrane with Different Pore Width

Figures 8–10 show the mean squared displacement of carbon dioxide and nitrogen molecules perpendicular to the membrane in the membrane pores with different sizes. From these figures, it can be clearly seen that the mean squared displacements of nitrogen molecules are always higher than those of carbon dioxide molecules in the different systems. In other words, these results show that the diffusion rate of nitrogen is usually larger than that of carbon dioxide generally under the conditions. And, this advantage of nitrogen in the diffusion rate can overcome its inferior position in loading in some cases. This is why nitrogen can possess a higher permeance than carbon dioxide under some specified conditions. However, there is some

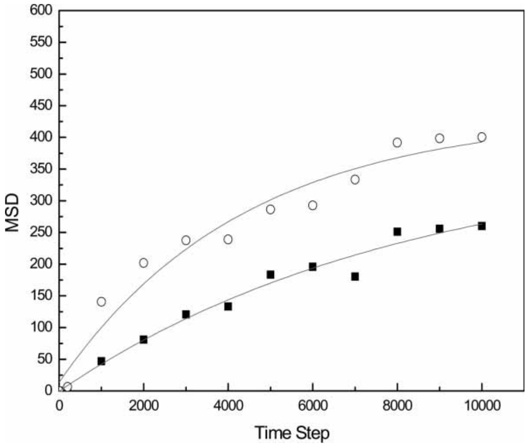

Figure 8. Mean squared displacement of CO_2 (■) and N_2 (○) in the pore of 0.4 nm.

difference about the slope of MSDs of carbon dioxide and nitrogen molecules with the increasing of time in the three figures. At short times, the slope of nitrogen is always higher than that of carbon dioxide from the three figures, but the status has been changed for a long time. For investigating the difference in detail, the diffusion coefficient *D* can be estimated from Figs. 8–10 through using Einstein's equation when time step is from 6000 to 1000. The diffusion coefficients are summarized in Table 2. From Table 2, it is found that the diffusion coefficient of nitrogen is still much higher than that of

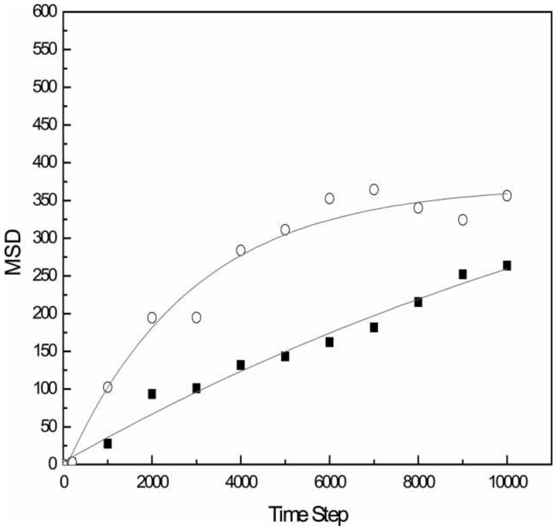

Figure 9. Mean squared displacement of CO_2 (■) and N_2 (○) in the pore of 0.66 nm.

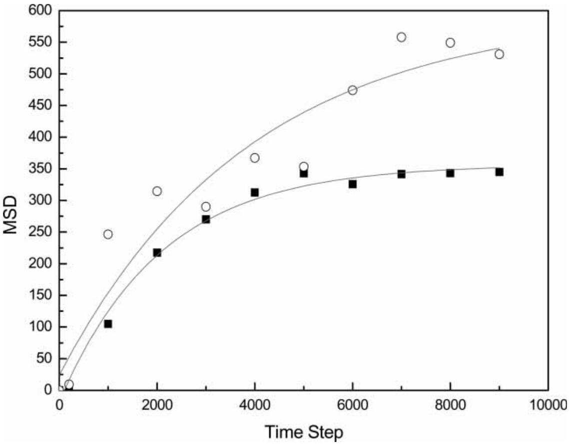

Figure 10. Mean squared displacement of CO_2 (■) and N_2 (○) in the pore of 1.0 nm.

carbon dioxide with increase of time when the pore size is 10 nm, however close to that of carbon dioxide in the pore with 0.4 nm. But in Fig. 9, we can see the diffusion coefficient of nitrogen is much lower than that of carbon dioxide and close to zero when the pore size is 0.66 nm. These phenomena indicates that the diffusion coefficients of nitrogen and carbon dioxide molecules may be influenced by the surface of pore wall along with the diffusion of gas molecules in the membrane pore. Confirmed by Fig. 6, nitrogen and carbon dioxide take on the different adsorption state in membrane pore. Thus, the diffusion coefficient of carbon dioxide adsorbed in a single layer can be larger than that of nitrogen adsorbed in two layers. Due to the predominance of the loading and the diffusion coefficient, the combination of the two effects produces the maximum of equilibrium selectivity of carbon dioxide when the membrane pore size is 0.66 nm. From the above analysis, it can be concluded that the surface diffusion of the gas molecules plays a key role in the separation process of carbon dioxide and nitrogen through carbon membrane. And, the effects of pressure and composition on

Table 2. Diffusion coefficient of CO_2 and N_2 in the different pore

Pore size (nm)	0.4	0.66	1.0
$D_{CO_2} \times 10^8$ ($m^2\ s^{-1}$)	2.60	3.01	0.60
$D_{N_2} \times 10^8$ ($m^2\ s^{-1}$)	3.76	0.0005	1.61

the equilibrium selectivity are imposed by the combination of the surface diffusion and the loading.

CONCLUSION

By means of the MC simulation in a relatively simple model, carbon membranes with slit-like pores at 300 k, the equilibrium selectivity of a CO_2/N_2 system under the different separation conditions is calculated. The simulation results demonstrate that the pore width is a key factor for the separation behavior of CO_2/N_2 mixture in the carbon membrane. When the pore width is 0.66 nm, a maximum of the equilibrium selectivity for carbon dioxide and nitrogen mixture system can be obtained.

Since the equilibrium selectivity of a CO_2/N_2 mixture lies on their adsorption capacity and diffusion in the membrane pore to a large extent, the density profiles and the mean squared displacement of carbon dioxide and nitrogen molecules in the membrane pores with the different pore width are investigated in detail in order to explore the microcosmic mechanism of the separation of a CO_2/N_2 mixture in the carbon membrane. The loading amount of carbon dioxide is always higher than that of nitrogen in membrane pores with different pore width, whereas the diffusion rate of nitrogen is higher than that of carbon dioxide in general. When the pore width is 0.66 nm, carbon dioxide and nitrogen molecules are adsorbed in terms of the different adsorption structure in the membrane pore so that the diffusion coefficient of carbon dioxide molecules is larger than that of nitrogen along with the diffusion in the membrane pores. Thus, a maximum of the equilibrium selectivity of carbon dioxide is obtained. The simulation results suggest that the surface diffusion of CO_2/N_2 mixture is very important for their separation in the carbon membrane.

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