

Gas separation effect of the pump driven by the thermal edge flow

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Abstract. The gas separation effect of the thermal edge compressor, which is a newly devised pump without moving parts driven by the thermal edge flow, is investigated numerically by the DSMC method based on the Boltzmann equation for a binary mixture of gases. Not only the separation of the species of the gas but also a molecular exchanging flows are observed in the thermal edge compressor. The numerical simulation is carried out for three intermolecular potentials, the hard-sphere, Maxwell molecules, and Lennard-Jones 12-6 models. It is also found that Maxwell molecule fails to describe the behavior of the gas mixture in the thermal edge compressor.

Keywords: gas separation, kinetic theory of gases, thermal edge flow, thermal transpiration, Knudsen compressor, molecular model

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1. INTRODUCTION

One of the exciting topics in the rarefied gas dynamics related to the micro-channel is the development of the devices without a moving part that work as a pump by making use of the gas flows induced by the temperature field. Different scales, materials, and driving mechanisms have been proposed for the device. [1–3] The primary interest in the researches for these devices has been their performance as a pump such as the compression ratio and pumping speed, so that the performance for pure gases has been investigated. However, the gas to be evacuated is usually a mixture of two or more kinds of gases, and individual component gases may flow differently inside the device, because these devices make use of the gas rarefaction effect (the thermally induced flows). This consideration suggests the possibility of the device as a gas separator. Recently the authors investigated this possibility in the case of the Knudsen compressor [1, 2], which is the pump driven by the thermal transpiration flow induced by the temperature gradient along the channel walls, in [4]. In the reference the analysis is carried out by the use of the fluid-dynamic model that is systematically derived from the Boltzmann equation and is available for the entire range of the Knudsen numbers. It was clarified that a fairly large separation effect is obtained by the Knudsen compressor and that the Maxwell molecule fails to capture the gas separation effect.

In the present paper, we investigate the gas separation effect of the thermal edge compressor [3] on the basis of the Boltzmann equation by the direct simulation Monte-Carlo (DSMC) method [5]. The driving mechanism of the thermal edge compressor is different from that of the Knudsen compressor: it makes use of the flows induced by the temperature difference between the solid bodies put in the channel. It does not require the temperature gradient on the channel walls, which is essential for the Knudsen compressor. As in [4], we carry out the numerical analysis for three intermolecular potentials, that is, the hard-sphere, Maxwell molecules, and Lennard-Jones 12-6 models.

2. PROBLEM

The thermal edge compressor consists of a number of driving units connected in series. Figure 1 shows an model of the driving unit of the device used in the experiment [3]. We shall consider this geometry of the pump unit. The channel is equipped with a pair of two arrays of the plates, one is heated (temperature T_h) and the other is unheated (temperature T_c). The unit induces a one-way flow of the gas in the X_1 direction (X_1, X_2 : Cartesian space coordinates) if the mean free path of the gas is comparable to the distance D_h between the neighboring plates of the array.

We analyze the following two problems when the system is filled with a binary mixture of gases, say, A and B.

Problem I: One-way flow : Consider a steady flow induced in an infinite series of units shown in Fig. 1. That is, we analyze the gas flows assuming that the flow is periodic in X_1 direction with the period of the width of a unit D_w .

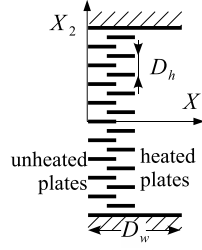


FIGURE 1. A unit of the thermal edge compressor.

Problem II: Closed system : Consider a pump system consisting of ten units, with both ends being choked by the unheated walls (temperature T_c). Initially the system is filled with uniform mixture of gases at rest. We investigate the time evolution of the behavior of the gas in the system.

The basic equation is the Boltzmann equation for a binary mixture:

$$\frac{\partial F^\alpha}{\partial t} + \xi_1 \frac{\partial F^\alpha}{\partial X_1} + \xi_2 \frac{\partial F^\alpha}{\partial X_2} = \sum_{\beta=A,B} J^{\beta\alpha}(F^\beta, F^\alpha), \quad (\alpha = A, B), \quad (1)$$

$$J^{\beta\alpha}(f, g) = \int_{|\xi_*| < \infty, 0 < b, 0 < \varepsilon < 2\pi} [f(\xi_*)g(\xi^{\beta\alpha}) - f(\xi)g(\xi_*)] |\mathbf{V}| b db d\varepsilon d\xi_*, \quad (2)$$

$$\xi^{\beta\alpha} = \xi + (m_*^{\alpha\beta}/m^\alpha)(\mathbf{V} \cdot \mathbf{a})\mathbf{a}, \quad \xi_*^{\beta\alpha} = \xi_* - (m_*^{\alpha\beta}/m^\beta)(\mathbf{V} \cdot \mathbf{a})\mathbf{a}, \quad \mathbf{V} = \xi_* - \xi, \quad m_*^{\alpha\beta} = 2m^\alpha m^\beta / (m^\alpha + m^\beta). \quad (3)$$

Here, the Greek characters α and β denote the gas species A or B; t is the time; ξ is the molecular velocity; m^α and F^α are the mass and the velocity distribution function of α -molecule; b and ε are the impact parameters of the molecular collision between α - and β -molecules[5]; \mathbf{a} is a unit vector determined by $\mathbf{V}, b, \varepsilon, m_*^{\beta\alpha}$, and the intermolecular potential $U^{\beta\alpha}(r)$ (r : the distance between the molecules). The following models of intermolecular potential are used:

(i) hard-sphere model (HS for short):

$$U^{\beta\alpha}(r) = \begin{cases} \infty, & [r < (d_m^{\alpha\alpha} + d_m^{\beta\beta})/2], \\ 0, & [r \geq (d_m^{\alpha\alpha} + d_m^{\beta\beta})/2], \end{cases} \quad (4)$$

(ii) Maxwell molecules (Maxwell for short):

$$U^{\beta\alpha}(r) = U_0^{\beta\alpha}/r^4, \quad (U_0^{\beta\alpha} = U_0^{\alpha\beta} : \text{Constants}), \quad (5)$$

(iii) Lennard Jones 12-6 model (LJ for short) [6]:

$$U^{\beta\alpha}(r) = 4k_B T_m^{\beta\alpha} \left[(d_m^{\beta\alpha}/r)^{12} - (d_m^{\beta\alpha}/r)^6 \right], \quad d_m^{\beta\alpha} = (d_m^{\alpha\alpha} + d_m^{\beta\beta})/2, \quad T_m^{\beta\alpha} = (T_m^{\alpha\alpha} T_m^{\beta\beta})^{1/2}, \quad (6)$$

where k_B is the Boltzmann constant, $(d_m^{\alpha\alpha}[\text{m}], T_m^{\alpha\alpha}[\text{K}])$ for LJ are the constants depend on species of the gas, e.g., $(2.576 \times 10^{-10}, 10.2)$ (He), $(2.789 \times 10^{-10}, 35.7)$ (Ne), and $(3.482 \times 10^{-10}, 122.4)$ (Ar). [7]

The boundary condition on the solid walls is the diffuse reflection:

$$F^\alpha(\xi \cdot \mathbf{n} > 0) = \sigma_w^\alpha \left(\frac{m^\alpha}{2\pi k_B T_w} \right)^{3/2} \exp\left(-\frac{m^\alpha |\xi|^2}{2k_B T_w}\right), \quad \sigma_w^\alpha = - \left(\frac{2\pi m^\alpha}{k_B T_w} \right)^{1/2} \int_{\xi \cdot \mathbf{n} < 0} \xi \cdot \mathbf{n} F^\alpha d\xi, \quad (7)$$

where T_w and \mathbf{n} are, respectively, the temperature and the unit normal vector to the boundary, pointed to the gas.

The macroscopic quantities are defined by the moments of the velocity distribution function F^α as follows:

$$n^\alpha = \int_{|\xi| < \infty} F^\alpha d\xi, \quad \mathbf{v}^\alpha = \frac{1}{n^\alpha} \int_{|\xi| < \infty} \xi F^\alpha d\xi, \quad \chi^\alpha = n^\alpha / n, \quad (8)$$

$$n = \sum_{\alpha=A,B} n^\alpha, \quad \mathbf{v} = \sum_{\alpha=A,B} m^\alpha n^\alpha \mathbf{v}^\alpha / \sum_{\alpha=A,B} m^\alpha n^\alpha, \quad 3k_B n T = \sum_{\alpha=A,B} m^\alpha \int_{|\xi| < \infty} |\xi - \mathbf{v}|^2 F^\alpha d\xi, \quad p = k_B n T, \quad (9)$$

where n , \mathbf{v} , T , and p are the molecular number density, flow velocity, temperature and pressure of the mixture, respectively. Those quantities with superscript α represent those for α -gas, and χ^α is the molar fraction of α -gas.

To complete the physical condition of the Problems I and II, the amounts of each molecule in the domain under consideration are required. Here we introduce \bar{n}^α , the average molecular number density of α -gas in a period (Problem I) or in the system (Problem II). The overall molar fraction $\bar{\chi}^A$ of A-gas is then defined by

$$\bar{\chi}^A = \bar{n}^A / (\bar{n}^A + \bar{n}^B). \quad (10)$$

3. METHOD OF ANALYSIS

We analyze the system of equations (1)–(7) numerically by the DSMC method from an appropriate initial condition. The numerical method is essentially the same as that explained in [1], where HS molecule is considered. The main difference between the numerical method for HS and that for other models is that the integrand in Eq. (2) vanishes except $0 < b < (d_m^{\alpha\alpha} + d_m^{\beta\beta})/2$ in HS and it does not generally vanish except $b \rightarrow \infty$ in other models. Therefore we introduce a cut-off of b to save the computational time. The criterion of the cut-off is determined by referring the effect of the collision, that is, the value of $\cos \theta = \mathbf{V} \cdot \mathbf{a} / |\mathbf{V}|$. We introduce variables (w, g) instead of $(|\mathbf{V}|, b)$:

$$(w, g) = \begin{cases} \left(m_*^{\alpha\beta} |\mathbf{V}|^2 / 4U_0^{\beta\alpha}, w^{1/4}b \right), & \text{(Maxwell),} \\ \left(m_*^{\alpha\beta} |\mathbf{V}|^2 / 16k_B T_m^{\beta\alpha}, [w^2 / (1+w)]^{1/12} (b/d_m^{\beta\alpha}) \right), & \text{(LJ).} \end{cases} \quad (11)$$

For Maxwell molecules, θ depends only on g and is nondecreasing. On the other hand, for LJ model, θ depends on g and w ; it converges to 0 as $g \rightarrow 0$ and $\pi/2$ as $g \rightarrow \infty$, and it diverges on a curve $g = g(w)$ [$g(w) = 1.3 \sim 1.4, w < 0.2$] which corresponds to the trajectory to the orbit formed by the attractive force. For these models, the cut-off $g < g_0 = 2$ is applied here. In this case $|\cos \theta|$ of the collisions neglected is smaller than 0.065 for Maxwell and 0.025 for LJ. The functional form of $\theta(g, w)$ for LJ is obtained only numerically.

The size of g_0 is related to the definition of the mean free path. In this paper the reference mean free path ℓ_0^{AA} , by which the Knudsen number Kn is defined as $\text{Kn} = \ell_0^{AA} / D_h$, is that for pure A-gas at equilibrium state $F_e^A(\boldsymbol{\xi})$ at rest with temperature T_c and molecular number density n_0 :

$$\ell_0^{AA} = \begin{cases} 1 / \sqrt{2} \pi n_0 (d_m^{AA})^2, & \text{(HS),} \\ n_0 \left(\frac{8k_B T_c}{\pi m^A} \right)^{1/2} \left[\frac{\pi}{g_0^2} \int_{|\boldsymbol{\xi}| < \infty, |\boldsymbol{\xi}_*| < \infty} \left(\int_0^{g_0} F_e^A(\boldsymbol{\xi}) F_e^A(\boldsymbol{\xi}_*) \frac{\partial b^2}{\partial g} dg \right) |\mathbf{V}| d\boldsymbol{\xi} d\boldsymbol{\xi}_* \right]^{-1}, & \text{(Maxwell and LJ).} \end{cases} \quad (12)$$

The mean free path ℓ_0^{AA} defined by Eq. (12) does not vanish in the limit $g_0 \rightarrow \infty$. In this paper, the molecular number density n_0 is taken equal to the number density of the mixture $\bar{n}^A + \bar{n}^B$.

Here we add a note on the parameters related to the intermolecular potentials. In the case of pure A-gas, there is only one parameter d_m^{AA} (HS) or U_0^{AA} (Maxwell), while there are two parameters d_m^{AA} and T_m^{AA} for LJ. As the result, the nondimensional form of the Boltzmann equation for LJ model contains two parameters, Kn and T_m^{AA}/T_c , while that for HS or Maxwell contains Kn only. For a binary mixture, there are more parameters related to B-molecules. That is, d_m^{BB}/d_m^{AA} for HS; U_0^{AB}/U_0^{AA} and U_0^{BB}/U_0^{AA} for Maxwell; T_m^{BB}/T_c and d_m^{BB}/d_m^{AA} for LJ. In this paper, we assume $d_m^{BB}/d_m^{AA} = 1$ for HS, $U_0^{AB}/U_0^{AA} = U_0^{BB}/U_0^{AA} = 1$ for Maxwell. For LJ, the values of T_m^{AA}/T_c , T_m^{BB}/T_c , and d_m^{BB}/d_m^{AA} are calculated from the corresponding values of $(d_m^{\alpha\alpha}, T_m^{\alpha\alpha})$ for each species under the condition $T_c = 300[\text{K}]$.

4. RESULTS

4.1. One-way flow

We first show the results for Problem I. The computation is carried out for $T_h/T_c = 3$ and several pairs of $(\text{Kn}, \bar{\chi}^A)$ tabulated in Table 1. The mass ratio m^B/m^A is 10 for HS and Maxwell. For LJ, the case $(A, B) = (\text{He}, \text{Ar})$ ($m^B/m^A = 9.98$) are considered. The values of “average” velocity defined by the ratio of total momentum to the total mass of α -gas

$$\bar{v}_1^\alpha = \int_S n^\alpha v_1^\alpha dX_1 dX_2 / \int_S n^\alpha dX_1 dX_2, \quad (13)$$

TABLE 1. Average flow velocity \bar{v}_1^α (Problem I). The case with $T_h/T_c = 3$, $m^B/m^A = 10$ and $d_m^{BB}/d_m^{AA} = 1$ for HS; A: He, B: Ar, and $T_c = 300[\text{K}]$ ($m^B/m^A = 9.98$) for LJ; $m^B/m^A = 10$ and $U^{AA} = U^{BB} = U^{AB}$ for Maxwell.

model	(Kn, χ^A)	$\frac{\bar{v}_1^A}{(2k_B T_c/m^A)^{1/2}}$	$\frac{\bar{v}_1^B}{(2k_B T_c/m^A)^{1/2}}$	model	(Kn, χ^A)	$\frac{\bar{v}_1^A}{(2k_B T_c/m^A)^{1/2}}$	$\frac{\bar{v}_1^B}{(2k_B T_c/m^A)^{1/2}}$
HS	(0.5, 0.2)	0.012	0.013	LJ	(0.1, 0.5)	0.007	0.007
HS	(0.5, 0.5)	0.016	0.016	LJ	(0.5, 0.5)	0.017	0.016
HS	(0.5, 0.8)	0.025	0.025	LJ	(2, 0.5)	0.016	0.014
HS	(0.5, 0.95)	0.031	0.028	Maxwell	(0.1, 0.5)	0.012	0.011
HS	(0.15, 0.5)	0.012	0.012	Maxwell	(0.5, 0.5)	0.023	0.016
HS	(1.5, 0.5)	0.014	0.014	Maxwell	(2, 0.5)	0.020	0.008

at steady state are shown in Table 1, where S is the area of a unit of the pump. Although the mass ratio is about 10, the difference of the average flow velocities between species is small except several cases for Maxwell molecules. The gas separation effect of the pump is considered to be small under this condition, but this is a special case without average pressure gradient along X_1 axis. The result also indicates that the collisions between A- and B-molecules are not negligible at the Knudsen numbers where the pump induces large flow velocity without the average pressure gradient.

4.2. Closed system

Next we show the results for Problem II, the time evolution of the mixture in the closed pump system consisting of ten units. For later convenience we number the units $i = 1, 2, \dots, 10$ from smaller to larger X_1 .

First we present the result for the case with $T_h/T_c = 3$, $\chi^A = 0.5$, and $\text{Kn} = 0.5$. The other parameters are the same as those in Sec. 4.1. The time evolution of the spatial distribution of pressure p of the mixture and molar fraction χ^A is shown in Fig. 2 in the case of HS model. The time evolution of \bar{v}_1^α [Eq. (13) with S being replaced by the total area of the system], the unit-average of the molecular number density \bar{n}_i , and that of the molar fraction χ_i^A [$\bar{h}_i = \int_{S_i} h dX_1 dX_2 / \int_{S_i} dX_1 dX_2$ ($h = n, \chi^A$; S_i : the area of i -th unit)] for HS, LJ, and Maxwell are compared in Fig. 3.

We will discuss the behavior of the gas in the case of HS based on Figs. 2 and 3(a). In $t/t_0 \lesssim 800$ [$t_0 = D_h(2k_B T_c/m^A)^{-1/2}$], a gas flow is induced in X_1 direction [see \bar{v}_1^α of Fig. 3(a)]. This flow is due to the one-way flow induced by the device. The flow is blocked by the walls at both ends of the system, and it induces a pressure gradient in X_1 direction [Fig. 2(a) $t/t_0 = 250 \sim 300 \rightarrow 950 \sim 1000$]. Then the flow decreases by the pressure gradient. The behavior of \bar{v}_1^α of Fig. 3(a) indicates that the effect of pressure gradient is larger for A-gas; that is, \bar{v}_1^A decreases

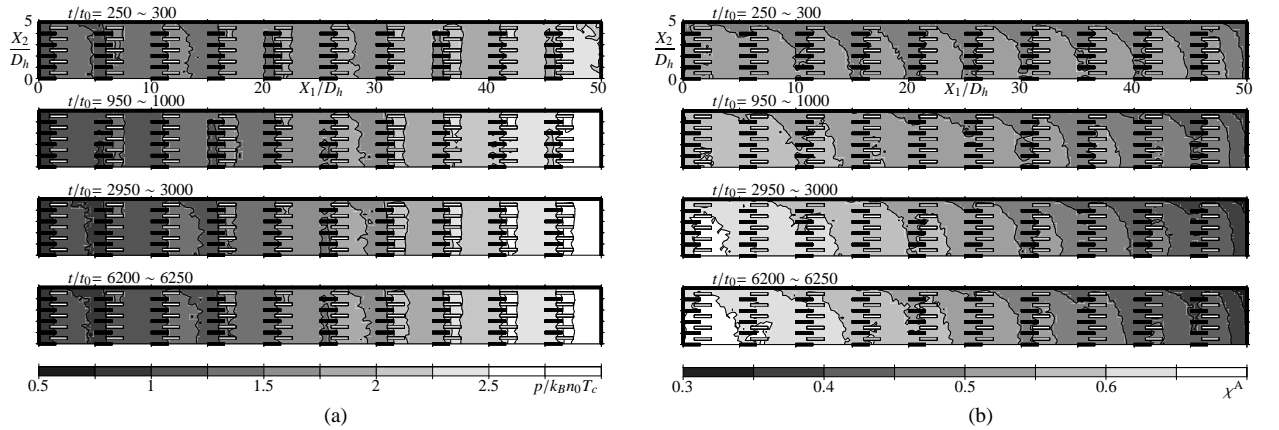


FIGURE 2. Time evolution of the pressure and the molar fraction in the system (Problem II). (a) Pressure p and (b) molar fraction χ^A are shown by the shade of darkness. The case with $T_h/T_c = 3$, $\text{Kn} = 0.5$, $\chi^A = 0.5$, and HS model with $m^B/m^A = 10$ and $d_m^{BB}/d_m^{AA} = 1$. $t/t_0 = 250 \sim 300, 950 \sim 1000, 2950 \sim 3000$, and $6200 \sim 6250$. Only the part for $X_2 > 0$ is shown here because of the symmetry with respect to $X_2 = 0$.

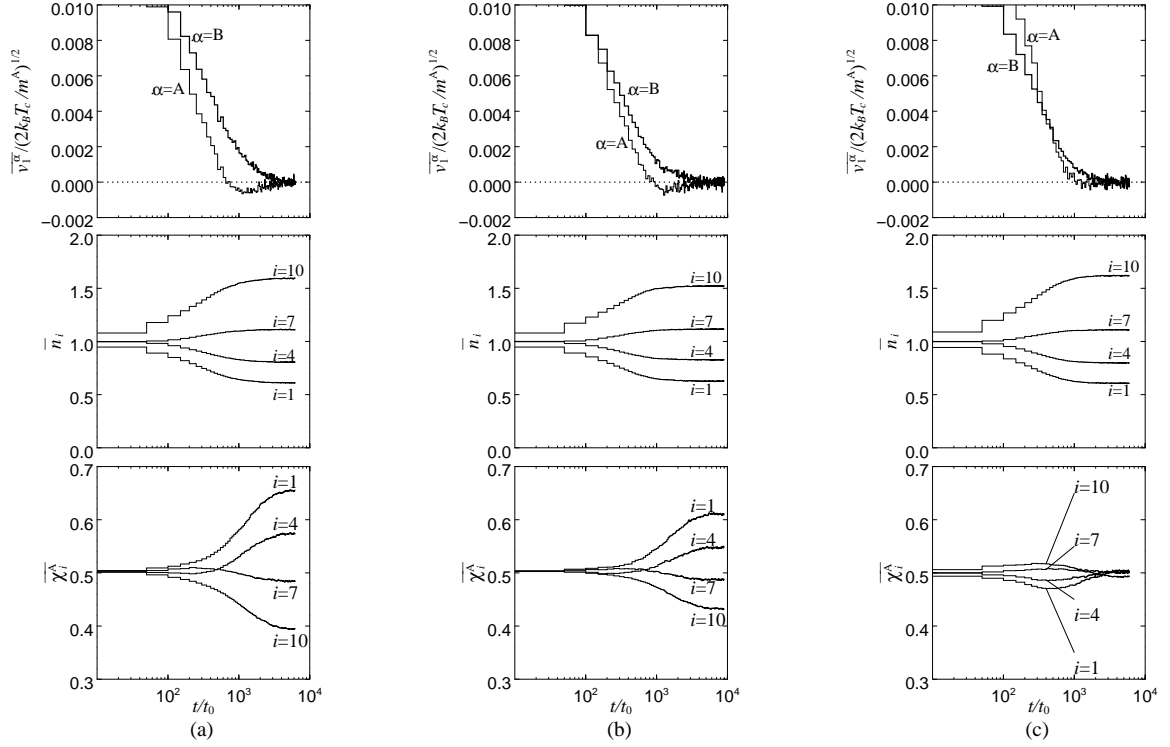


FIGURE 3. Time evolution of the average flow velocity $\overline{v_1^\alpha}$, the molecular number density $\overline{n_i}$ and the molar fraction $\overline{\chi_i^A}$ ($i = 1, 4, 7$, and 10) averaged over each area of unit- i for HS, LJ, and Maxwell models. $T_h/T_c = 3$, $\text{Kn} = 0.5$, and $\overline{\chi^A} = 0.5$. (a) HS, (b) LJ, and (c) Maxwell (see the caption of Table 1).

faster than $\overline{v_1^B}$. The average flow velocity of A-gas vanishes at $t/t_0 \sim 800$ while that of B-gas is still positive. The difference of the flow velocity induces a concentration gradient in the system [Fig. 2(b) $t/t_0 = 950 \sim 1000$ and $\overline{\chi_i^A}$ of Fig. 3(a)]. At time $1000 \lesssim t/t_0 \lesssim 3000$, where the pressure and molecular number density (thus also the temperature) of the mixture are roughly time-independent [see Fig. 2(a) and $\overline{n_i}$ of Fig. 3(a)], A-gas flows in $-X_1$ direction, and B-gas flows in X_1 direction. The development of the concentration gradient during the corresponding time is due to this molecular exchanging process. The molecular exchanging process ceases after sufficient concentration gradient has been established [Fig. 2(b) $t/t_0 = 950 \sim 1000 \rightarrow 6200 \sim 6250$, $\overline{v_1^\alpha}$ and $\overline{n_i}$ of Fig. 3(a)]. The difference of molar fraction $\overline{\chi_1^A} - \overline{\chi_{10}^A}$ between the both ends of the system at the steady state is 0.26.

The qualitative feature of the time evolution for LJ model [Fig. 3(b)] is the same as that for HS. The difference of the molar fraction at the steady state is slightly smaller than that of HS; that is, $\overline{\chi_1^A} - \overline{\chi_{10}^A} = 0.18$ for LJ.

For Maxwell molecules [Fig. 3(c)], the average flow velocity for A-gas is larger than that of B-gas in $t/t_0 \lesssim 500$ (cf. Table 1), but their order of the size reverses around $t/t_0 \sim 500$. Therefore, a concentration gradient once induced around $t/t_0 \sim 500$ is cancelled later. Only a little concentration gradient is left at the steady state.

The numerical analysis is also carried out for various sets of Kn and $\overline{\chi^A}$ in the case with $T_h/T_c = 3$. The obtained steady state is shown in Fig. 4. In the figure, the filled circle indicates Kn and $\overline{\chi^A}$, and a series of ten hollow circles nearby indicates the local Knudsen number Kn_i and $\overline{\chi_i^A}$ ($i = 1, 2, \dots, 10$), where Kn_i is defined by the unit-average of the molecular number density $\overline{n_i}$ and temperature $\overline{T_i}$ of the mixture. The shift of Kn_i represents the pumping effect and that of $\overline{\chi_i^A}$ represents the separation effect. A fairly large separation effect is observed for HS [Fig. 4(a)] and LJ [Fig. 4(b)] for the intermediate Knudsen numbers, whereas only a little separation effect is observed for Maxwell molecules [Fig. 4(c)].

The gas separation effect is also observed for other cases with different mass ratios. In the case of LJ, $T_h/T_c = 3$, $\text{Kn} = 0.5$, and $\overline{\chi^A} = 0.5$, the difference of molar fraction $\overline{\chi_1^A} - \overline{\chi_{10}^A}$ at the steady state is 0.16 for (A, B) = (He, Ne) ($m^B/m^A = 5.04$) and 0.08 for (Ne, Ar) ($m^B/m^A = 1.98$).

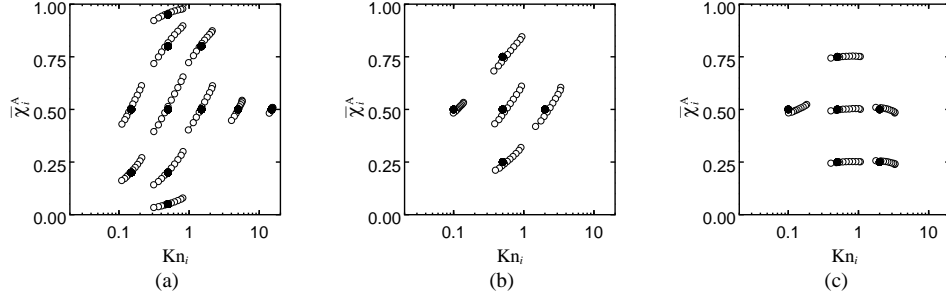


FIGURE 4. The the local Knudsen number Kn_i and the molar fraction $\bar{\chi}_i^A$ of i -th unit ($i = 1, 2, \dots, 10$) in the system at the steady state. $T_h/T_c = 3$. \circ : $(\text{Kn}_i, \bar{\chi}_i^A)$ ($i = 1, 2, \dots, 10$), \bullet : $(\text{Kn}, \bar{\chi}^A)$. (a) HS, (b) LJ, and (c) Maxwell (see the caption of Table 1).

The parameters for DSMC computation in this section is as follows. The gas region is divided into uniform square cells of the size $(D_h/4, D_h/4)$. The total number of simulation particles is 1.6×10^6 . The time step Δt is $5 \times 10^{-3} t_0$. The computations with cell size $(D_h/8, D_h/8)$ and 6.4×10^6 simulation particles are also carried out for several cases, and it is confirmed that there is no significant change on the distribution of \bar{n}_i and $\bar{\chi}_i^A$ at steady state.

5. CONCLUDING REMARKS

We investigated the behavior of a binary mixture of gases in the thermal edge compressor by the DSMC method using three kinds of intermolecular potentials, the hard-sphere, Maxwell molecules, and Lennard-Jones models. As in the preceding analysis[4], the qualitative feature of the result for Maxwell molecule differs from those for hard-sphere and Lennard-Jones models. Since Lennard-Jones model is the most reliable model among them, we conclude that Maxwell molecule fails to describe the behavior of the gas mixture in the thermal edge compressor. This result, together with that in [4], shows the incapability of Maxwell molecule in describing a physical phenomena at intermediate Knudsen numbers. These results should be distinguished from the well-known incapability of the model for the thermal diffusion in the continuum regime[6].

The results for the hard-sphere and Lennard-Jones models show that the present model of the thermal edge compressor has a gas separation effect at intermediate Knudsen numbers. The individual flow velocities of the component gases are almost the same in the one-way flow (Sec. 4.1), but they are different from each other in the closed system after an average pressure gradient along the system is established (Sec. 4.2). A molecular exchanging process, where the gas with smaller molecular mass flows from high pressure part to low pressure part and the other gas flows in the opposite direction, is observed. Since the molecular exchanging flow is blocked by the walls at the both ends of the system, a fairly large concentration gradient along the system is induced at the steady state.

One may find a similarity between the present results and the porous membrane gas separation which makes use of the Knudsen diffusion. In both cases the gas with smaller molecular mass has larger flow velocity in the opposite direction of the pressure gradient. The driving force of the porous membrane separation is the pressure gradient given by some external device. On the other hand, the pressure gradient in the present system is induced by itself. If the pressure gradient in the present system is given by some external device, we have a freedom to set the direction of individual flows of the component gases of the mixture by controlling the power of the pump device.

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