Free-molecular gas flow through the high-frequency oscillating membrane

V L Kovalev¹,², A N Yakunchikov¹,² and V V Kosiantchouk¹,²

¹ Institute of Mechanics, M.V. Lomonosov Moscow State University, Michurinskii prosp. 1, Moscow 119192, Russian Federation
² Department of Mechanics and Mathematics, M.V. Lomonosov Moscow State University, Leninskie Gory 1, Moscow 119991, Russian Federation

E-mail: vasily.kosyanchuk@gmail.com, art-ya@mail.ru

Abstract. The possibility of using a high frequency oscillating track membranes as diffusion membranes for gas separation was studied. High frequency forced oscillation of the membrane was considered because of assumption that the membrane conductivity for a given gas can be controlled by varying the frequency and amplitude of oscillation. The problem about free-molecular gas flow through a oscillating in its plane membrane was stated and the possibility of separation of gases using such a device was investigated. Also, optimal values of membrane oscillation parameters for most efficient gas separation have been found.

1. Introduction

Membrane technologies are widely used in many areas of space industry nowadays. Applications for membranes in space include: lunar and planetary habitats, RF reflectors and waveguides, optical and IR imaging, solar concentrators for solar power and propulsion, sun shades, solar sails and many others [1, 2]. Other important application is the construction of novel separation devices working in microgravity [3]. The problem with modern membrane separation technologies is that they use membranes “as is” and the performance of any membrane separator is based only on the properties (physical or chemical) of membrane material.

In recent years, many researches discovered novel physical effects caused by external impacts such as optical radiation [4], temperature gradient [5] and induced oscillations [6] on gas flow in microstructures where gas is flowing in rarefied regime. The influence of all these effects on the flow of multicomponent gas mixtures was shown to lead to mixture separation.

In authors previous papers [7, 8] a novel effect of gas separation using track membranes oscillating with high frequency was discovered; it was shown, that varying the amplitude and frequency of oscillations one can control the conductivity of the membrane for the given gas, and as a result, achieve the effect of gas separation. The purpose of the present work is to determine optimal values of membrane oscillation parameters for the most efficient gas separation.

2. Problem Statement

Multicomponent gas flow through the oscillating in its plane membrane, consisting of straight cylindrical channels of length L and radius R is considered. Membrane connects two volumes with constant pressures — p₁, p₂, and constant temperatures — T₁, T₂ (Fig.1) Temperatures of
the gas in volumes are equal and coincide with the temperature of the membrane \( T_1 = T_2 = T_w \), where \( T_w \) — is the temperature of membrane). Membrane moves as absolutely rigid body and the law of motion of each channel axis is as follows: \((x, y) = (x_c, y_c + Asin(\omega t + \psi))\), where \( x_c, y_c \) — initial coordinates of channel axis (which is directed along \( z \)), \( A \) and \( \omega \) — amplitude and frequency of oscillations. It is assumed that the influence of gas flow on the motion of membrane can be neglected. Temperature of channel wall is assumed to be constant in time and along channel axis. Molecules are modelled as material points, mass forces and internal degrees of freedom are neglected. Gas flow in channel is assumed to be free-molecular and the velocity distribution of molecules entering from volumes is equilibrium corresponding to volume temperature. Interaction of gas molecules with channel surface is described in terms of scattering kernel. For specific combination of gas and membrane material, the parameters of the kernel (and the scattering model itself) can be obtained from molecular dynamics trajectories computations \([9, 10, 11]\). The choice of the theoretical model to describe scattering in a number of problem appears to be fundamental. For example, the use of specular-diffusion Maxwell model in the problem of thermal transpiration leads to results qualitatively different from experiments \([12]\), and the Cercignani-Lampis scattering kernel does not allow the dependence of the energy and momentum conservation coefficients on the energy of incident gas molecules \([13]\). In the present work, calculations were conducted using Maxwell scattering kernel with full energy and impulse accommodation which is the extreme case for all scattering models.

Figure 1. Problem scheme: 1, 2 — tanks, separated by track membrane, oscillation direction shown by arrow (\( y \)-axis).

3. Computations
Problem was studied using event-driven molecular dynamics method \([14]\). For detailed description, please refer to \([7]\). Assumption that all membrane channels are equal and membrane moves as absolutely rigid body implies that flow can be studied only in one channel. Assumption about the free-molecular flow regime allows to simplify modelling to sequential computations of trajectories independently for each molecule. The computation was as follows. The same way as in \([7]\), coordinate and velocity of a new gas molecule at the inlet section of the channel were calculated according to given distributions. Then, the point of collision between gas molecule and channel wall was calculated. After that, a new velocity of molecule was calculated according to the scattering kernel and then a new point of collision was calculated. This continued up until molecule leaved the channel.
4. Results

Studied model has five defining parameters \( R, L, A \) — radius, length and amplitude of channel oscillations, \( \omega \) — oscillation frequency, \( v_m = \sqrt{\frac{2kT}{m}} \) — most probable thermal speed of gas molecules (where, \( k \) — boltzmann constant, \( T \) — volume temperature, \( m \) — mass of gas molecule). The problem was solved using dimensionless variables for simplicity of computations and analysis of results. Presented model has only two dimensions — length and time. Thus, parameters \( R, v_m \) were chosen for nondimensionalization:

\[
 r' = \frac{r}{R}, \quad A' = \frac{A}{R}, \quad L' = \frac{L}{R}, \quad u' = \frac{u}{v_m}, \quad t' = \frac{tv_m}{R}, \quad \omega' = \frac{\omega R}{v_m},
\]

where \( r, u, t \) — coordinate, velocity and time, \( r', u', t' \) — their dimensionless analogues.

According to \( \pi \)-theorem, passing probability \( P \) is a function of three dimensionless combinations, composed of five defining parameters. These combinations were chosen as follows. Dimensionless channel length, dimensionless oscillation amplitude and the ratio of characteristic oscillations speed to characteristic thermal speed of molecules:

\[
 L' = \frac{L}{R}, \quad A' = \frac{A}{R}, \quad c = \frac{A\omega}{v_m},
\]

During the simulations, these combinations were changed in the ranges \((5–500; 0,1–10; 0–7)\). Further the stroke indices are omitted and the use of dimensionless variables is assumed.

4.1. Effect of gas separation

The values of the parameter \( c \) depend on the characteristic speed of the molecules, and, therefore, are not equal for different gases. Thus, the stronger probability \( P \) depends on \( c \), the more will be the difference between values of membrane conductivity for different gases. To study the influence of oscillations on membrane conductivity \( P \), its value in the figures is normalized by the calculated probability of passing a static channel \( P_0(L) \) (as we are primarily interested in how much the passing probability decreases in oscillating channel in comparison with the static one), which is in a good agreement with Clausing’s empirical formula [15, 16]:

\[
P_0(L) = \frac{1 + 0.4L}{1 + 0.95L + 0.15L^2}.
\]

Further, we deal with already normalized dependency \( P(L, A, c) \).

Fig.2 shows dependencies \( P(c) \) at \( L = 5 \) for different values of \( A \). The decreasing behaviour of \( P(c) \) represent the effect of gas separation. Indeed, consider two species of gas with masses of molecules \( m_1, m_2 \). Given parameters of membrane oscillations, two values of parameters \( c_1, c_2 \) and different passing probabilities \( P(L, A, c_1), P(L, A, c_2) \), correspond to these masses. As passing probabilities are different for two gases, the molecular flow through membrane will differ too which will result in gas separation.

4.2. Determination of optimal parameters

Note that values \( c_1, c_2 \) mentioned above are related as follows

\[
k = \frac{c_1}{c_2} = \frac{v_{m_2}}{v_{m_1}} = \sqrt{\frac{m_1}{m_2}}.
\]

Without loss of generality, assume that \( P(L, A, kc) > P(L, A, c) \). Then for a given \( k \) the values of parameters \( L, A, c \) will be optimal for gas separation if the ratio of membrane conductivity for two gases — \( P(L, A, kc)/P(L, A, c) \) reaches its maximum.
As one can see from Fig.2, a at $A > 1$ probability $P(c)$ monotonically decreases as $A$ decreases from 10 to 1. Thus, the conductivity decreases most rapidly with increase of $c$ at $A = 1$. As is seen from Fig.2, b at $A < 1$ and small values of $c$ ($c < 0.8, 4$) probability $P(c)$ decreases most rapidly at the smallest value of $A$ ($A = 0, 2$). However, when $c$ increases, the monotony on $A$ breaks and at big values of $c$ the minimal value of $P(c)$ is again reached at $A = 1$.

Thus, the value of amplitude $A = 1$ is optimal for gas separation since membrane conductivity at this value of $A$ decreases most as $c$ increases. Calculations showed that this conclusion is also valid for other values of $L$. Fig.3, a shows dependencies $P(c)$ at $A = 1$ for values $L = 5, 10, 20, 50$. Note, that curves for different values of channels length are identical to the stretching along the $c$ axis, i.e. dependency $P(L, c)$ has the form $P(f(L) \cdot c)$. It can be shown that in this case variation of channel length does not increase the effectiveness of separation. Indeed, if for length $L$ maximum ratio of membrane conductivities for two gases is reached at some value $c_0$

$$c_0 = \text{arg max} \frac{P(f(L) \cdot kc)}{P(f(L) \cdot c)} \quad (L, k - \text{const})$$

then for any other length $L'$ one can achieve the same ratio setting $c'_0 = (f(L) \cdot c_0)/f(L')$. At the same time, there is no such value $c'_1$ for length $L'$, which would give greater ratio than $c'_0$. Otherwise, turning back to $L$, and setting $c_1 = (f(L') \cdot c'_1)/f(L)$, we get the ratio of conductivities, greater than at $c$, which stands in contradiction with the original assumption.

It is seen from Fig.3, a that the value $c$ required to achieve the equivalent level of conductivity decreases as $L$ grows. Hence, the value of oscillation speed required to obtain maximal effect of gas separation also decreases. Fig.3, b shows points of the curves from Fig.3, a, after stretching of each of them with its own coefficient $f(L)$ along $c$ axis. One can obtain this coefficient from Fig.3, a , for instance: $f(5) = 1; f(10) = 1.21; f(20) = 1.35; f(50) = 1.47$. As seen from Fig.3, b, all the points fit to one curve. Equation of the approximation curve is

$$P(c) = \frac{1 + 0.4c^{3.75}}{1 + 0.41c^{2.75} + 0.25c^{4.76}}. \quad (1)$$

Using dependency 1, one can find optimal value of parameter $c$ for any $L$ as an argument of maximum of the function

$$g(c) = \frac{P(f(L) \cdot kc)}{P(f(L) \cdot c)}.$$
5. Conclusions
Problem was solved numerically by event-driven molecular dynamics method. Passing probability was obtained in dependence on dimensionless parameters. It was shown that varying the frequency and amplitude of oscillation can lead to difference of membrane conductivity for gases with different molecular mass. This means that one can control the conductivity of the membrane for a given gas by changing the parameters of its forced oscillations.

Also, for separation of binary gas mixtures in free molecular flow by the means of an oscillating membrane:

(i) The optimal amplitude of membrane oscillation was found.
(ii) Approximation for the dependence of membrane conductivity on the dimensionless oscillation speed was constructed, which allows to determine the optimal value of oscillation speed.
(iii) It was shown that variation of the channel length does not increase efficiency of gas separation but allows to reduce the required speed of membrane oscillation.

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