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Study of gas separation by the means of high-frequency membrane oscillations

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ABSTRACT

The study of a free-molecular flow through the membrane oscillating in its own plane has been conducted. 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]. In authors' previous papers [4,5] 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 — p_1, p_2, and constant temperatures — T_1, T_2 (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: $(x, y) = (x_c, y_c + A\sin(\omega t + \psi))$, where x_c, y_c — initial coordinates of channel axis (which is directed along z), A and ω — 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

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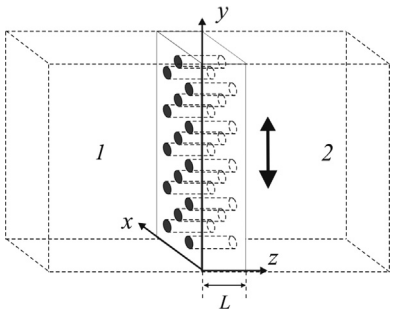

Fig. 1. Problem scheme: 1, 2 — tanks, separated by track membrane, oscillation direction shown by arrow (*y*-axis).

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 [6–8]. 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 [9], 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 [10]. 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.

3. Computations

Problem was studied using event-driven molecular dynamics method [11]. For detailed description, refer to [4]. 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 [4], 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, ω — oscillation frequency, $v_m = \sqrt{2kT/m}$ — 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:

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

where $\mathbf{r}, \mathbf{u}, t$ — coordinate, velocity and time, $\mathbf{r}', \mathbf{u}', t'$ — their dimensionless analogues. According to π-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. 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. 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 passing probabilities $P(L, A, c_1)$, $P(L, A, c_2)$, correspond to these masses. Note that values c_1, c_2 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.

5. Determination of optimal parameters

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 $P_0(L)$, which is in a good agreement with Clausing's empirical formula [12,13]:

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

Further, we deal with already normalized dependency $P(L, A, c)$. Fig. 2 shows dependencies $P(c)$ at $L = 5$ for values $A = 1, 2, 5, 10$ (a), and for values $A = 1, 0.8, 0.5, 0.2$ (b). As is seen 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 $A < 1$ small values of c ($c < 0.4$) probability $P(c)$ decreases most rapidly at the smallest