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THE INFLUENCE OF AN EXTERNAL FIELD ON THE SPATIAL DISTRIBUTION OF GAS PARTICLES EMERGING FROM A CYLINDRICAL CHANNEL

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The effect of an external field on the spatial distribution of particles emerging from a cylindrical channel has been investigated with adsorption and surface diffusion of particles on the channel walls taken into consideration.

The spatial distribution of particles emerging from channels is very important in studies of interaction of gas molecules with a solid surface and in development of molecular beam generators [1, 2]. A required spatial distribution of gas molecules leaving a cylindrical channel is usually achieved by choosing an appropriate channel length-to-radius ratio (in the case of impermeable walls) [2]. The spatial distribution can also be controlled by changing the physicochemical conditions on the channel walls, which can destroy the particles [3]. The possibility of controlling the angular distribution of molecules leaving a cylindrical channel by varying the inner channel surface, where a chemical reaction destroying the particles occurs, was discussed in [4]. The authors of [5] investigated the formation of a molecular beam by prescribing a temperature drop along a channel with an evaporating inner surface. In [6] the situation where phase changes occurred on part of the channel surface, whereas the rest of the surface area was not covered by condensate, was considered. This study was carried out to investigate whether an external field, changing the mode of interaction of gas particles with the surface, influences the spatial distribution of particles emerging from a cylindrical channel. A rarefied gas flow in narrow channels can be substantially influenced by surface diffusion of particles adsorbed on the channel walls [7], and surface diffusion also changes the angular distribution of particles leaving the channel [8]. In this case it appears possible to control the adsorbate distribution along the channel length and, accordingly, the net flow of particles emerging from the channel by external fields changing the mode of interaction between the gas particles and the surface. So, in [9] radiation-induced mass transfer in channels was investigated and in [10] the problem of initiating mass transfer by an electric field was considered. It is known that an adsorbed particle (an atom or a molecule) often has properties different from those inherent in the particle in the gas phase. In particular, the wall can "induce" an electric charge or a dipole moment in an adsorbed particle [11]. Thus, in the presence of an electric field, directed motion of adsorbed particles can arise on the channel surface. The particle flow density can be written as follows

$$j_s = -D_s \frac{dn_a}{dX} + bn_a F,$$

where D_s is the surface diffusion coefficient; n_a is the adsorbed particle density; F is the force caused by the action of the external field on an adsorbed particle; b is the mobility of an adsorbed particle ($b = D_s/kT$, where T is the channel surface temperature and k is the Boltzmann constant). The surface flow arising induces redistribution of absorbed particles on the channel surface and gives rise to a net flow of particles in the system, which is in equilibrium until the field is switched on [10]. The gas flow in the channel is assumed to be free molecular. For simplicity the adsorbed layer will be assumed to be rather rarefied so that Henry's law is satisfied for the adsorbed

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phase, and D_2 and the adsorption time τ can be taken to be independent of the adsorbed particle density in the first approximation. Desorbed particles are assumed to be distributed according to a cosine law.

With the above assumptions, n_a on the inner surface of a cylindrical channel of length L and radius R will be found from the equations (written in terms of the dimensionless coordinate x = X/L) [12]

$$\frac{1}{L^2}\frac{d}{dx}\left(D_s\frac{dn_a}{dx}-LbFn_a\right)=\frac{n_a}{\tau}-\alpha\left[\int_0^1\left(\frac{n_a}{\tau}+I\right)K_1(|x-x'|)\,dx'+\right.$$

$$\left.+N_0K(x)+N_1K(1-x)\right], \tag{1}$$

$$I=(1-\alpha)\left[\int_0^1\left(\frac{n_a}{\tau}+I\right)K_1(|x-x'|)\,dx'+N_0K(x)+N_1K(1-x)\right],$$

where α is the sticking coefficient; K and K_1 are functions characterizing the probability of passage of a particle from one surface element to another [1]; N_0 and N_1 are the flow densities of particles entering the channel at x = 0 and x = 1, respectively.

With the characteristic length at which equilibrium n_a occurs assumed to be $(D_s\tau)^{1/2}$, the boundary conditions for Eq. (1) can be written as [12]

$$\left(D_s\frac{dn_a}{dx}-LbFn_a\right)\Big|_{x=0}=L\left(\frac{D_{s0}}{\tau_0}\right)^{1/2}[n_a(0)-\alpha\tau_0N_0], \tag{2}$$

$$\left(D_s\frac{dn_a}{dx}-LbFn_a\right)\Big|_{x=1}=L\left(\frac{D_{s1}}{\tau_1}\right)^{1/2}[\alpha\tau_1N_1-n_a(1)], \tag{3}$$

where subscripts 0 and 1 on τ and D_s refer to their values at the end faces at x = 0 and x = 1.

The right-hand side of Eq. (1) describes the difference between desorbing and adsorbing particles.

Let us consider the particle distribution over a substrate located normal to the channel axis at a distance H from its outlet. A contribution to the flow of particles incident on the substrate will be made by particles desorbed from the channel walls and falling on the substrate without intermediate collisions with the walls, particles coming from the channel inlet, and particles desorbed from the end face at the outlet section. The two first components (denoted by I_1 and I_2) are calculated as follows [8]:

$$I_1=\frac{2l^2}{\pi}\int_{x_0}^1\int_{\beta}^{\pi}(1-\rho\cos\omega)\frac{n_a}{\tau}\frac{(1+h-x)\,d\omega dx}{[l^2(1+h-x)^2+1+\rho^2-2\rho\cos\omega]^2},$$

where $\rho = r/R = H\tan\theta/R$ is the ratio of the distance r between the channel axis and the point on the substrate considered and the channel radius; θ is the angle between the straight line connecting the center of the outlet section with the given point on the substrate and the channel axis; $l = L/R$ is the dimensionless length of the channel; h = H/L. In this case the lower integration limits x_0 and β depend on the interval in which the angle θ, corresponding to the substrate region considered, occurs:

$$\text{At}\quad \theta\leqslant\theta_A,\ \text{where}\ \theta_A=\operatorname{arctg}\left(\frac{1}{lh}\right):\quad x_0=0,\ \beta=0;$$

$$\text{at}\quad \theta_A<\theta\leqslant\theta_B,\ \text{where}\ \theta_B=\operatorname{arctg}\left(\frac{2h+1}{lh}\right):\quad x_0=0,$$

$$\beta=\beta_1=\arccos\left[\frac{2h-(1-x)(\rho^2-1)}{2\rho h}\right];$$

$$\text{at}\quad \theta_B<\theta\leqslant\frac{\pi}{2}:\quad x_0=1-\frac{2h}{\rho-1},\ \beta=\beta_1.$$

The expression for the azimuthal angle β_1 at a certain channel cross section x = const is determined starting from the fact that it characterizes the limiting point on the inner surface, from which molecules can reach the vicinity of the given point on the substrate (at smaller angles ω this is prevented by screening by the channel wall):

$$I_2 = \frac{N_0}{2}\left\{1 - \frac{\rho^2 - 1 + l^2(1+h)^2}{\sqrt{(1-\rho)^2 + l^2(l+h)^2[l^2(1+h)^2 + 2(1+\rho^2)]}}\right\}$$

at $\theta < \theta_A$ and

$$I_2 = \frac{2N_0}{\pi} l^2(1+h)^2 \iint\limits_{S_0} \frac{\eta d\eta d\omega}{[l^2(1+h)^2 + \rho^2 + \eta^2 - 2\rho\eta\cos\omega]^2}$$

at $\theta_A < \theta \leq \theta_B$, where S_0 is the bottom area (dimensionless), visible from the point r on the substrate. The expression for the component of the flow density due to particles falling on the substrate after desorption from the end face at the outlet section, has the form [8]

$$I_3 = \frac{1}{\pi}\int\limits_S \frac{n_a}{\tau} \frac{h^2 \bar{r} d\bar{r} d\omega}{[h^2 + h^2\,\mathrm{tg}^2\theta + \bar{r}^2 - 2h\bar{r}\,\mathrm{tg}\,\theta\cos\omega]^2},$$

where $\bar{r} = r/L$ and integration is carried out over the area A of the annulus from which the particles desorb.

In what follows, it is assumed for simplicity that the density of adsorbed particles on the end face changes linearly from n_a of (1) to zero (the channel ends in a vacuum and particles that can reach the end face after escaping from the substrate are also neglected).

For calculation of the flows I_1, I_2, and I_3, it is necessary to find n_a from Eq. (1). When seeking an approximate solution for n_a, the conditions q, E, τ, D_S = const, $G = \tau D_S/L^2 << 1$, $\varphi = \tau bF/L << 1$ are assumed to be satisfied. When the parameters G, $\varphi << 1$, the differential terms in (1) will influence the adsorbate distribution in the channel only within narrow boundary layers near its ends and in the region where these terms can be neglected, in an exponential approximation of the functions K and K_1 under the indicated conditions, it is possible to obtain for $(n_a/\tau) + 1$ the expression

$$\frac{n_a}{\tau} + I = Ax + B, \tag{4}$$

where

$$A = (N_1 - N_0)\frac{lx}{l+2}, \quad B = \frac{N_0(l+1)}{l+2} + \frac{N_1}{l+2}.$$

When $N_1 = 0$, we have

$$\frac{n_a}{\tau} + I = -\frac{N_0 lx}{l+2} + \frac{N_0(l+1)}{l+2}. \tag{5}$$

In order to find an approximate solution of Eq. (1), Eq. (5) will be substituted into the integrand in (1) [12]. Then, for n_a we have the equation

$$\frac{d^2 n_a}{d^2 x} - \frac{\varphi}{G}\frac{dn_a}{dx} - \frac{1}{G}n_a = -\frac{\alpha\tau}{G}\left[N_0\frac{l+1}{l+2} - \frac{N_0 l}{l+2}x\right],$$

the solution of which has the form

$$n_a = C_1\exp\{s_1 x\} + C_2\exp\{s_2 x\} + N_0\alpha\tau\left\{\frac{l+1}{l+2} - \frac{l}{l+2}(x-\varphi)\right\}, \tag{6}$$

where

$$s_{1,2} = \frac{\varphi \pm (\varphi^2 + 4G)^{1/2}}{2G}.$$

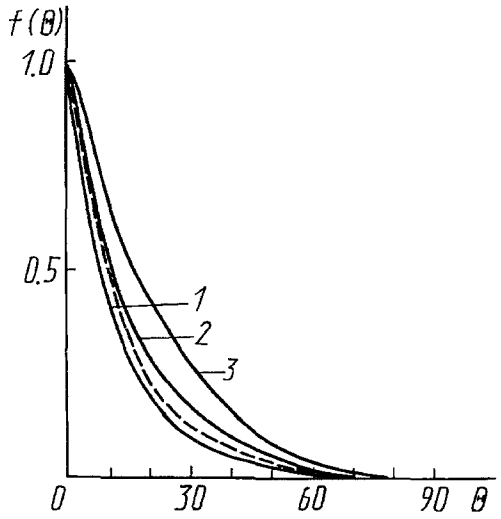

Fig. 1. Plot of the particle distribution over the substrate versus F for the case $D_s = D_{s0} = D_{s1}$, $\tau = \tau_0 = \tau_1$ for $D_s\tau = 10^{-8}$ cm^2; $l = 10$; $\alpha = 1$, h = 10; T = 500 K; L = 10^{-3} cm; 1) F = $-8\cdot10^{-10}$ dyne; 2) 0; 3) $8\cdot10^{-10}$.

The coefficients C_1 and C_2 are found from the set of equations obtained from (6) and boundary conditions (2) and (3):

$$\left[D_s s_1 - LbF - L\left(\frac{D_{s0}}{\tau_0}\right)^{1/2}\right] C_1 + \left[D_s s_2 - LbF - L\left(\frac{D_{s0}}{\tau_0}\right)^{1/2}\right] C_2 =$$

$$= L\left(\frac{D_{s0}}{\tau_0}\right)^{1/2}\left[N_0\alpha\tau\left(\frac{l+1+l\varphi}{l+2}\right) - \alpha\tau_0 N_0\right] +$$

$$+ \frac{D_s N_0 \alpha\tau l}{l+2} + LbFN_0\alpha\tau\frac{l+1+l\varphi}{l+2},$$

$$\left[D_s s_1 - LbF + L\left(\frac{D_{s1}}{\tau_1}\right)^{1/2}\right]\exp\{s_1\} C_1 + \left[D_s s_2 - LbF + L\left(\frac{D_{s1}}{\tau_1}\right)^{1/2}\right] \times$$

$$\times \exp\{s_2\} C_2 = -L\left(\frac{D_{s1}}{\tau_1}\right)^{1/2} N_0\alpha\tau\left(\frac{l\varphi+1}{l+2}\right) +$$

$$+ \frac{D_s N_0\alpha\tau l}{l+2} + LbFN_0\alpha\tau_0\frac{l\varphi+1}{l+2}.$$

The dimensionless flow density of particles incident on the substrate $f(\theta)$, which characterizes the spatial distribution of the particles, is determined by summing I_1/N_0, I_2/N_0, and I_3/N_0. In Fig. 1 results are presented for $f(\theta)$ calculated for the case $D_s = D_{s0} = D_{s1}$ and $\tau = \tau_0 = \tau_1$ (note that here $f\theta$ depends only on the product $D_s\tau$, and not on D_s and τ separately [8]). For comparison, in Fig. 1 the curve for a channel with an impermeable surface neglecting surface diffusion (the dashed line) is also shown. As folllows from the above calculations, the force F can either broaden or narrow the spatial distribution of the particles, depending on its direction. When the field-induced particle flow coincides in direction with that caused by surface diffusion, the spatial distribution is broadened (curve 3). If the force F is directed oppositely, under its action adsorbed particles will be displaced along the wall toward the inlet, because of which the inner surface of the channel adjacent to the outlet section will contain a smaller number of particles and the spatial distribution of the particles will be narrowed (curve 1). It should be noted that the surface diffusion effect with the external field neglected will result in broadening of the spatial distribution relative to the spatial distribution of particles leaving a cylindrical channel without surface diffusion (curve 2). The field effect can result in spatial distributions smaller than those in the case considered (surface diffusion can be a factor that will provide narrower molecular beams).

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