EFFECT OF THE ATTRACTIVE POTENTIAL OF THE WALLS ON THE FLOW OF A RAREFIED GAS IN A LONG THIN PLANE CHANNEL

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We consider the flow of a rarefied gas in the presence of attractive surface forces. It is shown that when the channel thickness is close to the range of the surface forces the gas flow is described by an equation which differs from the formula for free-molecular flow.

The average flux density ($i = Q/\pi r_0^2$) of a rarefied gas through a circular channel in the assumption of diffuse scattering of molecules by the walls is given by the Knudsen formula [1]

$$i = \frac{\Delta p}{\sqrt{2\pi mkT}} \frac{r_0}{L}, \; L \gg r_0. \tag{1}$$

The analogous formula for a plane channel ($i = Q/d$) is

$$i = \frac{\Delta p}{\sqrt{2\pi mkT}} \frac{d}{L} \ln \frac{2\sqrt{e}\,L}{d}, \; L \gg d. \tag{2}$$

Equations (1) and (2) are valid when the transverse dimensions of the channel are much smaller than the mean free path of a molecule in the gas:

$$\lambda_0 \gg r_0, \; \lambda_0 \gg d. \tag{3}$$

Deviations form (1) were observed experimentally in [2] for channels with very small transverse dimensions ($r_0 \sim 0.5$ µm). In such channels i no longer depends on r_0. Evidently this qualitative change in the nature of the flow is caused by the increased importance of the interaction of the gas with the walls, since in this case the range of the surface forces covers a significant fraction of the channel volume. A qualitative explanation of the result was given in [2] assuming that the scattering of gas molecules by the walls is described by the diffusely specular Maxwell model [1], and that the coefficient of accommodation vanishes for angles below a certain very small value. In addition, it was assumed that diffusely scattered molecules are not incident at such small angles. In [3, 4] the linear response method was used together with a numerical calculations to show that when the dimensions of the channel are decreased down to the range of the molecular interactions (~3-5 Å) the diffusion coefficient of the gas increases anomalously. The effect of nonequilibrium phonons in the channel walls on the gas flow was studied in [5, 6]. However, long-range dispersion forces were not taken into acocunt. The effects of adsorption and surface mobility on gas flow were studied in [7]. It was shown that in thin capillaries surface flow begins to play a major role and the flow deviates from Knudsen flow.

In the present paper we consider the effect of long-range surface attraction on the flow of a rarefied gas in a thin plane surface attraction on the flow of a rarefied gas in a thin plane channel. The treatment is based on the use of the Boltzmann equation and the assumption of diffuse scattering. The interaction potential of gas molecules with the walls is chosen as a rectangular well [8]

$$U(x, y, z) = \begin{cases} 0, & d_1 \leqslant z \leqslant d - d_1, \\ -U_0, & 0 < z < d_1, \; d - d_1 < z < d, \end{cases} \tag{4}$$
$$d > 2d_1,$$

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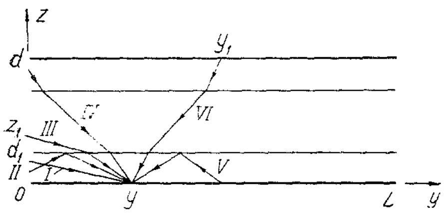

Fig. 1

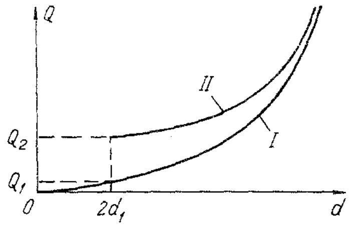

Fig. 2

Fig. 1. Types of trajectories of molecules arriving at a given point (y, z = 0) of the channel wall.

Fig. 2. Dependence of the flux Q on channel thickness d (solid curves): I) without attractive forces; II) with attractive forces $(Q_1 = 2pd_1^2 \ln (L\sqrt{e}/d_1)/L\sqrt{2\pi mkT},\ Q_2 = Q_1 \exp (U_0/kT))$.

here z is the coordinate perpendicular to the walls, y is the coordinate along the gas flow, and x is perpendicular to the gas flow in the plane of the walls. This rather crude model for the long-range attractive forces can only be used when the potentials of the opposing walls do not overlap. This means that all of the results obtained here are valid only when $d > 2d_1$.

The collisionless Boltzmann equation describing the rarefied gas has for its solution a distribution function which is invariant along the trajectories of motion between collisions with the walls [1]. For example, in the absence of interactions

$$f(\mathbf{r},\ \mathbf{v},\ t) = f(\mathbf{r} - \mathbf{v}(t - t_0),\ \mathbf{v},\ t_0). \tag{5}$$

We consider steady flow. Following [1, 9] we consider the Boltzmann equation subject to a boundary condition of the form

$$|\mathbf{vn}|\, f^+(\mathbf{r},\ \mathbf{v}) = \int\limits_{(\mathbf{v}'\mathbf{n})<0} d\mathbf{v}'\, W(\mathbf{v}' \to \mathbf{v})\, |\mathbf{v}'\mathbf{n}|\, f^-(\mathbf{r},\ \mathbf{v}'),\quad (\mathbf{vn}) > 0, \tag{6}$$

where the point r lies in the channel wall.

For diffuse scattering [1]

$$W(\mathbf{v}' \to \mathbf{v}) = |\mathbf{vn}|\, W_0(\mathbf{v}),\quad W_0(\mathbf{v}) = \frac{m^2}{2\pi (kT)^2} \exp\left(-\frac{m\mathbf{v}^2}{2kT}\right). \tag{7}$$

Then from (6) and (7) we obtain

$$f^+(\mathbf{r},\ \mathbf{v}) = J(\mathbf{r})\, W_0(\mathbf{v}), \tag{8}$$

where

$$J(\mathbf{r}) = \int\limits_{(\mathbf{v}'\mathbf{n})<0} d\mathbf{v}'\, |\mathbf{v}'\mathbf{n}|\, f^-(\mathbf{r},\ \mathbf{v}'). \tag{9}$$

Hence the problem reduces to the calculation of the function $J(\mathbf{r})$.

For a plane channel with identical walls the integral in (6) splits up into six integrals corresponding to the six types of trajectories along which a molecule can arrive at a given point y of the surface (Fig. 1).

Here for simplicity we assume that there is no gas at the right end of the channel. Along trajectories I-IV molecules arrive at point y directly form the end of the channel (y = 0) without collision with the walls. Using the invariance of the distribution along the trajectories, the function $f^-_{I-IV}(y,\ \mathbf{v}')$ can be expressed in terms of the given boundary distribution $f_0(z,\ \mathbf{v})$ at the end of the channel. For example, we have for trajectories of type III [8]

$$f^-_{III}(y,\ \mathbf{v}') = f_0(z_1,\ \mathbf{v}),$$

where

$$\mathbf{v}' = \{v_x',\ v_y',\ v_z'\};\ \mathbf{v} = \{v_x',\ v_y',\ -\sqrt{v_z'^2 - 2U_0/m}\};$$

$$z_1 = d_1(1 - \sqrt{1 - 2U_0/mv_z'^2}) + y\sqrt{v_z'^2 - 2U_0/m}\,/v_y',$$

and the transformation of the z-component of the velocity $v_z' \to \sqrt{v_z'^2 - 2U_0/m}$ corresponds to passing through the boundary of the potential well $z = d_1$.

Along the trajectories V and VI a molecule arrives at point y on the wall after colliding with the walls of the channel and hence f^- can be expressed in terms of the distribution f^+ and therefore $J(y)$, in view of (8). In particular

$$f^-_{VI}(y, \mathbf{v}') = f^+_{z=d}(y_1, \mathbf{v}'),$$

where

$$y_1 = y + 2d_1 v_y'/v_z' - \frac{(d - 2d_1)\, v_y'}{\sqrt{v_z'^2 - 2U_0/m}}, \quad v_z'^2 > 2U_0/m.$$

Expressing the function $f^-(y, \mathbf{v}')$ through $f_0(z, \mathbf{v})$ in each of the six regions of integration composing the region $v_z' < 0$ in (9), and using (8), we obtain an integral equation for $J(y)$:

$$J(y) = J_0(y) + \int_0^L K(y - y')\, J(y')\, dy'. \tag{10}$$

Here the term $J_0(y)$ is due to the contribution of trajectories of types I-IV, whereas the integral term is due to the contribution of trajectories of types V and VI. In deriving (10) the distribution function $f_0(z, \mathbf{v})$ was chosen to be a Maxwell–Boltzmann distribution. The expressions for $J_0(y)$ and the kernel $K(y - y')$ are quite complicated and will not be written out here.

Equations of the type (10) have been studied in detail in [1]. For a long channel ($L \gg d$) the approximate solution has the form [1]

$$J(y) = \frac{p}{\sqrt{2\pi mkT}} \exp\left(\frac{U_0}{kT}\right)(1 - y/L), \tag{11}$$

where p is the pressure in the volume from which the gas flows into the channel. Equations (11) and (8) and the invariance condition along the trajectories give the complete solution of the problem for gas flow in a thin plane channel with the effect of long-range attractive forces taken into account.

In order to compare with experiments we calculate the flux of gas Q discharged from the channel. The quantity Q for a channel of arbitrary length can be written in the form [1]:

$$Q = Q_{\text{in}} + \int_0^L dy \int_{\Omega^+(y)} |\mathbf{v}\cdot\mathbf{n}|\, f^+(y, \mathbf{v})\, d\mathbf{v}, \tag{12}$$

Q_{in} is the contribution to the flux of molecules passing through the entire channel without making collisions with the walls and is determined by the distribution function $f_0(z, \mathbf{v})$ at the entrance to the channel. The calculation shows that in a long channel ($L \gg d$) the quantity Q_{in} becomes logarithmically small in comparison with the in integral term in (12). This is natural, since the probability of a molecules passing through the entire channel without making a collision with the wall is extremely small in this case. The integral term on the right hand side of (12) represents the contribution to the flux Q from molecules reflected from the walls of the channel. The region of integration $\Omega^+(y)$ in velocity space v, is determined by the condition $\mathbf{v} \in \Omega^+(y)$, if a molecule reflected from the wall at point y with velocity reaches the channel outlet without colliding with the walls. The set of all trajectories satisfying this condition splits up into four types: I^+-IV^+, which are analogous to the trajectories I-IV in Fig. 1, but are directed toward the channel outlet. Carrying out the integrations over these subregions, the quantity Q can be reduced to quadratures. However, this expression is quite complicated; simple analytical expressions can be obtained in two limiting cases:

$$U_0/kT \ll 1,$$

$$Q \approx \frac{p}{\sqrt{2\pi mkT}} \frac{d^2}{2L} \ln \frac{2\sqrt{e}\, L}{d}; \tag{13}$$

$$\frac{L}{d}\sqrt{U_0/kT} \gg 1,$$

$$Q \approx \frac{p}{\sqrt{2\pi mkT}} \left[\frac{(d - 2d_1)^2}{2L} \ln \frac{2\sqrt{e}\, L}{d - 2d_1} + \right.$$

$$+\frac{a_1(d-2d_1)}{L}\exp\left(\frac{U_0}{2kT}\right)K_0\left(\frac{U_0}{2kT}\right)+\frac{2d_1^2}{L}\exp\left(\frac{U_0}{kT}\right)\ln\frac{L\sqrt{e}}{d_1}\Bigg]. \tag{14}$$

We see from (13) and (14) that in a wide channel ($d \gg 2d_1$) the attractive forces affect the flow only slightly. In a thin channel ($d \gtrsim 2d_1$) the attractive surface forces significantly change the nature of the flow and the effect is larger the deeper the potential well (Fig. 2). This result is qualitatively consistent with the experimental results [2]. The inclusion of long-range forces leads to another condition for the applicability of the free-molecular approximation: a restriction on the depth of the potential well. As a result of the Boltzmann distribution, the density of gas is higher inside the potential well than outside of it, and therefore the mean free path λ insider the well is smaller than that λ_0 outside of it. Because $\lambda \sim 1/n$ [10], we have

$$\lambda = \lambda_0 \exp(-U_0/kT). \tag{15}$$

Therefore the condition (3) transforms into two inequalities:

$$\lambda_0 \gg d - 2d_1,\ \lambda_0 \exp(-U_0/kT) \gg d_1, \tag{16}$$

which restricts the potential well depth. The opposite case, when the second inequality in (16) is not satisfied and the surface motion can be considered as hydrodynamic, was considered in detail in [7]. In order to obtain a more accurate comparison with experiment, it is necessary to consider gas flow in a thin circular channel and to take into account the nonequilibrium nature of the interaction of the gas with the walls [5, 6, 11]. It may also be necessary to consider a more realistic model of the potential of the dispersion.

NOTATION

d, thickness of the plane channel: d_1, potential well width; e, base of naturel logarithms; $f(\mathbf{r}, \mathbf{v}, t)$, distribution function of the gas; $f_0(z, \mathbf{v})$, boundary value of the distribution function at the end of the channel; f^- and f^+, distribution functions of molecules incident on the surface and scattered molecules; i, flux density of the gas; k, Boltzmann constant; L, channel length; m, mass of a gas molecule; $\mathbf{n}$ outward normal to the surface; p, gas pressure; Δp, pressure drop; Q, gas flux at the channel outlet; $\mathbf{r}$, position vector; r_0, radius of the circular channel; T, temperature; t, time; U_0, potential well depth; $\mathbf{v}'$ and $\mathbf{v}$, velocity of a molecule incident on the wall and scattered from the wall; $W(\mathbf{v}' \to \mathbf{v})$, scattering function of the gas; x, y, z, Cartesian coordinates; λ_0, mean free path of a molecule outside the range of the surface forces; λ, mean free path inside the potential well.

LITERATURE CITED

1. K. Cherchin'yani, Theory and Application of the Boltzmann Equation [in Russian], Moscow (1978).
2. B. V. Deryagin and N. N. Fedyakin, Studies of Surfaces Forces [in Russian], Moscow (1964); pp. 244-257.
3. L. A. Grivtsova, A. G. Grivtsov, N. V. Churaev, and L. F. Chuikova, Kolloidn. Zh., 44, No. 5, 969-976 (1982).
4. L. A. Grivtsova, R. M. Ergunov, N. V. Churaev, and L. G. Khazin, "On the diffusion of gas molecules in microcapillaries with discrete adsorption centers," Preprint IPM AN SSSR, No. 136, Moscow (1984).
5. D. V. Borman, S. Yu. Krylov, and A. M. Kharitonov, Pis'ma Zh. Eksp. Teor. Fiz., 11, No. 7, 430-434 (1985).
6. D. V. Borman, S. Yu. Krylov, and A. M. Kharitonov, Zh. Éksp. Teor. Fiz., 92, No. 5, 1668-1683 (1987).
7. N. V. Pavlyukevich, G. E. Gorelik, V. V. Levdanskii, et al., Physical Kinetics and Transport Processes in the Presence of Phase Transitions [in Russian], Minsk (1980).
8. J. A. Barker and D. J. Auerbach, Far. Disc. Chem. Soc., No. 80, 277-289 (1985).
9. R. G. Barantsev, Interaction of Rarefied Gases with Streamlined Surfaces [in Russian], Moscow (1975).
10. A. Isikhara, Statistical Physics [in Russian], Moscow (1973).
11. F. O. Goodman and H. Y. Wachman, Dynamics of Gas-Surface Scattering, Academic Press, New York (1976).