FLOW OF A RELAXED GAS IN THE VICINITY OF A SOLID SURFACE

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Behavior of a polyatomic relaxed gas in the vicinity of a solid surface was studied. The case in which the size of the relaxation zone exceeds considerably the mean free path between the elastic collisions (suppressed exchange of translational and internal energies) was considered. A smooth validity of the asymptotic expansion for the distribution function with defined assumptions was indicated. A solution for the zero-approximation equation and boundary conditions for the surface flow, based on this solution and generalized model for a diffusive gas reflection from the surface were derived. The latter problem was partially studied in [1] by the Grad method and in [2] in terms of an analysis of the temperature jump.

A kinetic equation for polyatomic gases was obtained by formal generalization of the Boltzmann equation in [3] (reference from [4]). Using the notation of [4], we write

$$\frac{df_i}{dt}=\frac{\partial f_i}{\partial t}+\mathrm{V}_i\frac{\partial f_i}{\partial \mathrm{x}}=\sum_{j,k,l}\int(f_k'f_e'-f_if_j)g_{ij}I_{ij}^{kl}(g,\theta,\Phi)\sin\theta\,d\theta d\Phi\,d\mathrm{V}_j \tag{1}$$

The index i denotes the inner quantum numbers $\{i_1, i_2, \ldots\}$ characterizing the internal state of a molecule. The intersections I_{ij}^{kl} are the binary collision characteristics. For $g_{ij} = g_{ii}'$ let $I_{ij}^{ij} \sim \sigma_1$, $I_{ij}^{kl} \sim \sigma_2$ and for $g_{ij} \neq g_{kl}$ $'I_{ij}^{kl} \sim \sigma_{12}$, σ_1 and σ_{12} can depend on i, j; for this case it is not difficult to generalize the arguments.

Usually $\sigma_1 \sim \sigma_2 \sim \sigma$. Henceforth we distinguish two cases:

a) easy exchange of translational and internal energies,

$$\sigma_{12} \sim \sigma \tag{2}$$

b) suppressed exchange

$$\sigma_{12} \ll \sigma \tag{3}$$

We reduce Eq. (1) to a dimensionless form. For this besides the normal characteristics terms we introduced the linear dimension L, which in case a) is a length, where the distribution function undergoes a characteristic change, and in the case b) $L = (n\sigma_{12})^{-1}$. In the case b) we obtain

$$\begin{aligned}\frac{df_i}{dt}&=\frac{1}{\varepsilon}\sum_{j,k,l}\int(f_k'f_l'-f_if_j)g_{ij}I_{ij}^{kl}\sin\theta\,d\theta\,d\Phi\,d\mathrm{V}_j+\\&+\sum_{j,k,l}{}'\int(f_k'f_l'-f_if_j)g_{ij}I_{ij}^{kl}\sin\theta\,d\theta\,d\Phi\,d\mathrm{V}_j=\frac{1}{\varepsilon}J_i+J_i'\ ;\end{aligned} \tag{4}$$

$\varepsilon = (n\sigma L)^{-1} \ll 1$, the sign Σ denotes the sum with respect to transitions, with $g = g'$, whereas the sign Σ' refers to transitions with $g \neq g'$. In the case a) Σ' is multiplied by ε^{-1}.

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The information on the interaction mechanism of polyatomic gases with a solid surface is usually confined to the accommodation coefficients and some adsorption features. For a simple gas a semiempirical model of mirror-diffusion reflection with different accommodation coefficients is a common approach. By defining the boundary conditions for (4), we use the general functional relation, but the actual calculations are carried out for a generalized reflection diffusion model.

At the solid surface the following conditions should be fufilled:

$$f_i^+ = \sum V_{ij} f_j^- \tag{5}$$

where the plus sign signifies the molecules leaving the surface, and the minus sign, those arriving at the surface; V_{ij} is the linear operator whose characteristics will be discussed below.

We shall seek the solution of Eq. (4) with condition (5) in the case $\varepsilon \to 0$. With the method described in [5] it is possible to separate the functional dependence of f_i on ε (due to a tedious calculation this derivation will not be presented). The function f_i, besides the terms, proportional to the powers of ε, contains terms that characterize the boundary effects and which are multiplied by $\exp\{-\varepsilon^{-1}|\mathbf{x}-\mathbf{x}_*|\}$, where $\mathbf{x}$ is the coordinate of the point considered, while $\mathbf{x}_*$ is the intersection coordinate of the molecule trajectories arriving at the point $\mathbf{x}$ from the surface. We introduce a local coordinate system at the surface by directing one of the axes along the normal to the surface $\mathbf{n}$. It can be shown (see [5]) that the influence of condition (5) is concentrated in the region

$$x_n \lesssim \varepsilon \tag{6}$$

This region is called the Knudsen layer. The presence of a multiplier of order $\exp[-x_n/\varepsilon]$ leads to the exponential absorption with $\varepsilon \to 0$ of the effect of the boundary on the distribution function in any fixed internal flow point. The presence of a major parameter in front of the first sum in (4) (separating the integrals and sums from the number of collisions when the energy of the translation motion of the particles does not exchange with the energy of the internal degrees of freedom) allows us to separate the fast and slow processes which determine the evolution of the successive approximations f_i for $\varepsilon \to 0$. The explicit form of the zero and first approximations of the distribution function for the surface flow were obtained in [6, 1] by different methods. The aim of the present work is to find a uniformly valid expansion of the distribution function (for the surface flow and in the Knudsen layer) with respect to a small parameter. To do this, following [7], we introduce a perturbed coordinate

$$y = \varepsilon^{-1} x_n \tag{7}$$

which is an argument of the distribution function.

By restricting ourselves to the stationary case, we write the Boltzmann equation in the form

$$\frac{df_i}{dt} + \frac{1}{\varepsilon} V_n \frac{\partial f_i}{\partial y} = \frac{1}{\varepsilon} J_i + J_i' \tag{8}$$

where

$$\frac{df_i}{dt} = \mathbf{V}_\tau \frac{\partial f_i}{\partial \mathbf{x}_\tau} + V_n \frac{\partial f_i}{\partial x_n} \tag{9}$$

When y takes a final value, we obtain the points of the Knudsen layer, when $y \to \infty$ ($\varepsilon \to 0$ with a fixed x_n) the region of the surface flow. We seek the solution of Eq. (8) in the form

$$f_i = \sum_n \varepsilon^n f_i^{(n)}(\mathbf{x}, y) \tag{10}$$

By inserting (10) into (8), for the successive approximations we have

$$V_n \frac{\partial f_i^{(0)}}{\partial y} = J_i(f_i^{(0)}, f_j^{(0)}) \tag{11}$$

$$V_n \frac{\partial f_i^{(1)}}{\partial y} = J_i(f_i^{(0)}; f_j^{(1)}) + J_i'(f_i^{(0)}; f_j^{(0)}) + J_i(f_i^{(1)}; f_j^{(0)}) - \frac{df_i^{(0)}}{dt} \tag{12}$$

where J_i is the integral of the elastic collisions, J_i' is the integral of the inelastic collisions.

Due to the linearity and the lack of dependence of the condition (5) on ε they are transposed without changes in the successive approximations. We shall show that the equations for $f_i^{(n)}$ with $y \to \infty$ develops into the equations for the successive approximations in the surface flow [6], i.e., we shall show the uniform validity of the expansion (10).

We introduce the notation

$$J_i = -\nu_i(f_j) f_i + K_i(f_k;\, f_\varepsilon) \tag{13}$$

where

$$\begin{aligned} \nu_i &= \sum_{jke} \int f_j g_{ij} I_{ij}^{ke} \sin\theta\, d\theta\, d\Phi\, d\mathbf{V}_j \\ K_i(f_k;\, f_e) &= \sum_{j,\,k,\,e} \int f_k' f_e' g_{ij} I_{ij}^{kl} \sin\theta\, d\theta\, d\Phi\, d\mathbf{V}_j \end{aligned} \tag{14}$$

We reduce Eqs. (11) and (12) to the form

$$V_n \frac{\partial f_i^{(m)}}{\partial y} = -\nu_i(f_j^{(0)}) f_i^{(m)} + \Phi_i^{(m)} \tag{15}$$

We can write (15) in the integral form for $V_n > 0$ and correspondingly $V_n < 0$

$$f_i^{(m)}(y) = f_i^{(m)}(0) \exp\left[-\frac{\nu_i}{V_n} y\right] + \int_0^y \frac{\Phi_i^{(m)}(z)}{V_n} \exp\left[-\frac{\nu_i}{V_n}(y-z)\right] dz \tag{16}$$

$$f_i^{(m)}(y) = -\int_y^\infty \frac{\Phi_i^{(m)}(z)}{V_n} \exp\left[-\frac{\nu_i}{V_n}(y-z)\right] dz \tag{17}$$

The $f_i^{(m)}(0)$ are selected in such a way that the boundary condition (5) is fulfilled. We find the limiting values of the integrals entering (16) and (17) for $y \to \infty$

$$A_1 = \int_0^y \frac{\Phi_i^{(m)}(z)}{V_n} \exp\left[-\frac{\nu_i}{V_n}(y-z)\right] dz$$

$$A_2 = \int_y^\infty \frac{\Phi_i^{(m)}(z)}{V_n} \exp\left[-\frac{\nu_i}{V_n}(y-z)\right] dz$$

With the substitution $z = yt$ we obtain

$$A_1 = y \int_0^1 \frac{\Phi_i^{(m)}(yt)}{V_n} \exp\left[-\frac{\nu_i}{V_n} y(1-t)\right] dt$$

$$A_2 = y \int_1^\infty \frac{\Phi_i^{(m)}(yt)}{V_n} \exp\left[-\frac{\nu_i}{V_n} y(1-t)\right] dt$$

The integrands in these integrals are considerably different from zero for large y only in the region $1 - t \sim 1/y$. Due to the multiplier y, A_1 and A_2 for $y \to \infty$ tend to a limiting value which is different from zero. Assuming boundedness and continuity at an infinitely remote point $\Phi_i^{(m)}$ and using the Laplace method [8], we obtain that for $y \to \infty$

$$A_1 \to \nu_i^{-1} \Phi_i^{(m)}(\infty), \qquad A_2 \to \nu_i^{-1} \Phi_i^{(m)}(\infty)$$

Hence it follows that

$$f_i^{(m)} \to \frac{\Phi_i^{(m)}(\infty)}{\nu_i}, \qquad \frac{\partial f_i^{(m)}}{\partial y} \to 0$$

By differentiating (15) with respect to y, we can show by the same method that a derivative of any order of $f_i^{(m)}$ with respect to y also tends to zero as $y \to \infty$. If Eqs. (11), (12), ..., are compared by setting

$\partial f_i^{(m)}/\partial y = 0$ with the equations for the superficial flow derived in [6], we obtain the uniform validity of the expansion (10).

Let us analyze the zero approximation (11) with the condition at the boundary ($y = 0$)

$$f_i^{(0)} = \sum_j V_{ij} f_j^{(0)} \tag{18}$$

The limiting solution ($y \to \infty$) of this problem is known; it satisfies the equation

$$J_i\,(f_i^{(0)};\ f_j^{(0)}) = 0$$

and is of the form [6]

$$f_i^{(0)} = n\left(\frac{m}{2\pi k T_1}\right)^{3/2} \frac{1}{z} \exp\left\{-\frac{mc^2}{2kT_1} - \frac{E_i}{kT_2}\right\} \tag{19}$$

where m is the molecular mass, T_1 is the temperature of the translational degrees of freedom, T_2 is the temperature of the internal degrees of freedom

$$z = \sum_i \exp\left\{-\frac{E_i}{kT_2}\right\}, \quad n = \sum_i \int f_i\,d\mathbf{v}$$

$$\mathbf{c} = \mathbf{v} - \mathbf{U}, \quad \mathbf{U} = \frac{1}{n} \sum_i \int f_i \mathbf{v}\,d\mathbf{v},$$

n, u, T_1, and T_2 are functions of the external coordinate x.

We calculate the integral

$$I = \sum_i \int_0^y \int_{(\mathbf{v})} V_n \frac{\partial f_i^{(0)}}{\partial y} [\ln f_i^{(0)} + 1]\,d\mathbf{v}\,dy \tag{20}$$

$$I = \sum_i \int_0^y \frac{\partial}{\partial y} \int_{(\mathbf{v})} V_n f_i^{(0)} \ln f_i^{(0)}\,d\mathbf{v}\,dy = \sum_i \int_0^y \int_{(\mathbf{v})} J_i(f_i^{(0)} : f_j^{(0)})\,[\ln f_i^{(0)} + 1]\,d\mathbf{v}\,dy \tag{21}$$

The symmetry of direct and inverse collisions provides the result known from the proof of the H theorem [4],

$$I \leqslant 0 \tag{22}$$

Furthermore

$$I = \sum_i \left[\int_{(\mathbf{v})} V_n f_i^{(0)} \ln f_i^{(0)}\,d\mathbf{v}\right]\Bigg|_{y=0}^{y} \tag{23}$$

From (11) and the conditions of no-flow at the surface, it follows that $u_n = 0$ for all y. Taking (19) into account we let $y \to \infty$ in (23)

$$I(y \to \infty) = -\sum_i \left[\int_{(\mathbf{v})} V_n f_i^{(0)} \ln f_i^{(0)}\,d\mathbf{v}\right]\Bigg|_{y=0} \tag{24}$$

We introduce the notation

$$\langle f_i\,(V_n)\rangle = f_i\,(-V_n), \quad f_i^{(0)} = f_{wi}\,\varphi_i, \quad P\,(\varphi_i) = \varphi_i\,(\ln \varphi_i + \ln f_{wi} - 1)$$

where f_{wi} is a positive function, even with respect to V_n, and independent of y, that satisfies the conditions (18). We specify the form of the operator V_{ij}. The relation (18) links the distribution function of molecules, reflected from the surface (we mark it with plus) with the distribution function of the incident (minus) molecules, and includes the information on the interaction mechanism of a gas with the surface. The operator V_{ij} can be represented in the form

$$\frac{1}{f_{wi}} V_{ij}(f_{wj}\varphi_j) = H_{ij}(\varphi_j^-) = \frac{1}{V_n f_{wi}} \int_{(V_{jn}<0)} |v_{jn}|\,T_{ij}(\mathbf{v}, \mathbf{v}_j)\,f_{wj}\varphi_j\,d\mathbf{v}_j \tag{25}$$

$$\varphi_i^+ = \sum_j H_{ij}\varphi_j^- \tag{26}$$

By taking into account the no-flow condition at the surface and the normalizing conditions of T_{ij} with respect to **v**, which can be written for any function of φ_i satisfying (26)

$$\sum_i \int_{(\mathbf{v})} V_n f_{wi}\varphi_i \, d\mathbf{v} = -\sum_i \int_{(V_n<0)} V_n f_{wi}(\langle\varphi_i^+\rangle - \varphi_i^-)\, d\mathbf{v} = 0 \tag{27}$$

we can write

$$I = \sum_{i=0}^{\infty} \int_{(V_n<0)} V_n f_{wi} \left\{ P\left[\left\langle \sum_j H_{ij}(\varphi_j^-) \right\rangle\right] - P(\varphi_i^-) \right\} d\mathbf{v} \tag{28}$$

By substituting $P(\varphi_i^-)$ for φ_i^- in (27), we have

$$\sum_i \int_{(V_n<0)} V_n f_{wi} \left\{ \sum_j \langle H_{ij}[P(\varphi_j^-)]\rangle - P(\varphi_i^-) \right\} d\mathbf{v} = 0 \tag{29}$$

Eliminating $P(\varphi_i^-)$ from (28) via (29) we finally obtain

$$I = \sum_i \int_{(V_n<0)} V_n f_{wi} \left\{ P\left[\left\langle \sum_j H_{ij}(\varphi_j^-) \right\rangle\right] - \sum_j \langle H_{ij}[P(\varphi_j^-)]\rangle \right\} d\mathbf{v} \tag{30}$$

For $\varphi > 0$, the second derivative of P with respect to φ is greater than zero, and consequently $P(\varphi)$ is a convex function. For convex functions the generalized inequality of Jentzen is valid:

$$P\left(\frac{\sum_j \int q_{ij}(t, x)\, \Phi_j(x)\, dx}{\sum q_{ij}(t, x)\, dx} \right) \leqslant \frac{\sum_j \int q_{ij}(t, x)\, P[\Phi_j(x)]\, dx}{\sum_j \int q_{ij}\, dx}$$

for any $q_{ij} \geq 0$.

Assuming

$$\langle q_{ij}\rangle = \frac{1}{V_n f_{wi}} |V_{jn}|\, T_{ij}(\mathbf{v}, \mathbf{v}_j)\, f_{wj}, \quad \Phi_j = \varphi_j^-$$

and considering that f_{wi} satisfies the condition (18), we obtain for $V_n \leq 0$

$$P\left[\left\langle \sum_j H_{ij}(\varphi_j^-) \right\rangle\right] \leqslant \sum_j \langle H_{ij}[P(\varphi_j^-)]\rangle \tag{31}$$

The inequality (31) together with $V_n \leq 0$ from (30) gives

$$I \geqslant 0 \tag{32}$$

From (32) and (22) it follows that for all y

$$I = 0 \tag{33}$$

The negative definiteness of expression [4]

$$\sum_i \int_{(\mathbf{v})} J_i(f_i^{(0)}; f_j^{(0)})\, [\ln f_i^{(0)} + 1]\, d\mathbf{v}$$

gives an equation for $f_i^{(0)}$ which holds for all y:

$$J_i(f_i^{(0)}; f_j^{(0)}) = 0 \tag{34}$$

From this it follows that function (19) is the unique solution for the problem (11), (18), while the parameters n, U, T_1, and T_2 are independent of y. Hence the uniqueness theorem, proven for a pure gas in [9],* is generalized for the case considered.

It should be pointed out that the assumption on the existence of f_{wi}, which is even with respect to v_n, is very important. Physically this assumption implies the existence of such a gas state near the surface in which the distribution of molecules incident to and outgoing from the surface is the same. For a model of mirror-diffusion reflection such a state is realized in equilibrium, while for other cases this assumption should be verified, since without it the considerations lose their validity. We also note that the existence of a unique solution for the zero approximation in the Knudsen layer narrows the scope of simulating the law for the interaction of a gas with a surface and proves the hypothesis, put forward in [10], that the models T_{ij} and f_i must agree near the solid surface.

In order to obtain the boundary conditions for the equations of the first approximation in surface flow [6], we construct the actual model of the V_{ij} operator. In [11] it was noted that the molecular mean free path in an adsorbed layer depends on the internal state of the molecule (the idea of an adsorption gas-dynamic laser arose from this). Furthermore, the short stay-time of the molecules in the adsorbed state and different relaxation rate of translational and internal energy leads to a known experimental difference between the accommodation coefficients of translational and internal energy. This information permits us to generalize the diffusion law of reflection by introducing different accommodation coefficients for the internal and translational energies of the molecules. We consider that the distribution of molecules reflected from the surface at y = 0 (i.e., for $V_n > 0$) can be written in the form

$$\begin{gathered} f_{wi} = n_w\left(\frac{m}{2\pi kT_{1w}}\right)^{3/2}\frac{1}{z_w}\exp\left\{-\frac{mv^2}{2kT_{1w}} - \frac{E_i}{kT_{2w}}\right\} \\ T_{1w} = \alpha\theta,\ T_{2w} = \beta\theta,\ z_w = \sum_i \exp\left(-\frac{E_i}{kT_{2w}}\right) \end{gathered} \tag{35}$$

where θ is the surface temperature, α and β are the corresponding accommodation coefficients, n_w is determined from the surface no-flow conditions. From (35) and solutions for the zero approximations in the Knudsen layer we have

$$\mathbf{u} = 0,\ T_1 = T_{1w} = \alpha\theta, \qquad T_2 = T_{2w} = \beta\theta \tag{36}$$

These conditions are similar to the normal conditions of adhesion in the dynamics of a viscous liquid. Refinement of the conditions (36) associated with the glide and temperature jump effects appears in considering the subsequent approximation in which it is required to solve the linear inhomogeneous integrodifferential equation (12).

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