

INTERACTION OF MOLECULAR FLOW FROM A POINT SOURCE WITH A CONTINUOUS MEDIUM

B. L. Paklin and A. K. Rebrov

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The results of numerical simulation of the transformation of a molecular beam into a diffusive flow are presented in this paper. The notion of the relaxation length L_r is introduced as the main characteristic of the relaxation zone. Quantitative analysis for model molecules in the form of hard spheres in the practically important range of the ratio m_1/m_2 of the molecular masses of the source and medium and of the ratio S of velocities reveals the peculiarities of the relaxation process. The general problem of a molecular source in a continuum flow calls for careful investigation.

Statement of the Problem. The basic theoretical results of the translational relaxation of a molecular ensemble are well known for uniform relaxation conditions and relaxation in shock waves. The behavior of the molecular beam injected into a background gas in a given state is a particular subject in the study of the translational relaxation from the standpoint of the beam transformation into a diffusive flow, which is the degradation of the inert motion of molecules. Some elements of such processes occur in shock waves of gas mixtures, but they are concealed by collective phenomena of gas mixture relaxation. One can formulate a general statement of the problem of relaxation of molecular source gas in a continuum flow. A more general statement covers problems of continuum gas dynamics and kinetic theory. To this field of investigations one can refer the paper [1] where the molecular beam disintegration was studied from the viewpoint of penetration of heavy molecules into a light background gas. In a wider sense, one may refer to investigations of the vaporization (condensation) kinetics [2].

The explanation of molecular source gas relaxation can find practical applications in the elaboration of different vacuum technologies: deposition of molecules by evaporation, localized atomization, mixing and separation of gases, and production of ultradispersed particles. The high-altitude rocket engine plume formation also belongs to phenomena of this nature.

In the present work, molecular beam disintegration was studied in a linear formulation, that is, without taking into account intercollisions of injected molecules. The numerical experiments were performed by the Monte Carlo method for the ratio between molecular masses of injected and background molecules in the range $1 \gg m_1/m_2 - m_1/m_2 \gg 1$ at speed ratio S from 0 up to ∞ , determined by the most probable speed of the background gas molecules. The algorithm of this approach has been described in [3].

A general and apparent feature of molecular beam relaxation processes is the presence of a nonequilibrium zone in the space around a beam source. In this zone the velocity distribution function of injected molecules transforms into a distribution function corresponding to the equilibrium distribution function at the temperature of the background gas. The velocity distribution function of the background gas was assumed to be undisturbed and at equilibrium (Maxwellian). The calculations were performed for a simple hard sphere model of intermolecular collisions. As a result of systematic computational experiments, data were obtained on the topology of the relaxation zone and on the location of a fictitious point source of injected molecules, which acts as a pole of their diffusion drift toward infinity. In the case where the source molecules have an isotropic Maxwellian velocity distribution (with zero mean mass velocity) the solution is

Kutateladze Institute of Thermophysics, Siberian Division, Russian Academy of Sciences, Novosibirsk 630090. Translated from *Prikladnaya Mekhanika i Tekhnicheskaya Fizika*, Vol. 36, No. 5, pp. 3-6, September-October, 1995. Original article submitted October 31, 1994.

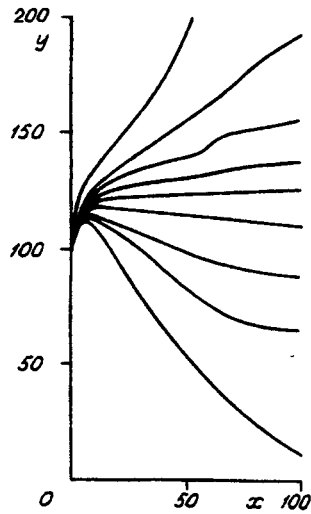


Fig. 1

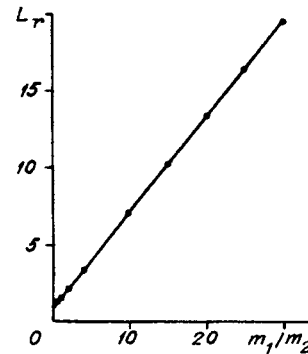


Fig. 2

the same as for the process of molecular effusion into a medium, which obeys the diffusion equation in the entire space except for the relaxation zone in the vicinity of the source.

We assume that the molecules of a point source are injected into the background gas in a selected direction with a certain velocity distribution function and that at infinity a spherical drift of molecules outward of the source with a fictitious center displaced off the real source exit occurs. To characterize this displacement, the notion of the mean length of decay of inertial molecular motion L_r is introduced below as a relaxation length. According to [4, 5], this length is the distance at which the molecular energy and momentum are persistent.

The relaxation length of the energy of injected molecules was determined as the mean path at which they acquire the mean energy corresponding to the temperature of the background gas, and the momentum relaxation length was determined as the mean molecular path at which the velocity component along the injection direction changes sign. The location of the point diffusive source depends on the relaxation length.

Analysis of the Computational Experiments. The main parameters on which the relaxation length can depend are the molecular mass m_1 of the source and of the background gas m_2 , the injection velocity V directed along the source axes, and the most probable velocity u of the background gas.

To study the dependence of L_r on these quantities, it is natural to use nondimensional parameters m_1/m_2 and $S = V/u$. The quantity $l = 1/n\sigma$ serves as a unit length (n is the numerical density of the background gas molecules, and σ is the collision cross section for the interaction of two types of molecules). For the model of interaction of molecules as hard spheres, one has $\sigma = \pi(r_1 + r_2)^2$, where r_1 and r_2 are the radii of source molecules and of background gas, respectively. The quantity $t = l/u$ serves as a unit time. A δ -function was taken as the velocity distribution function of injected molecules.

Figure 1 illustrates the averaged molecular flux from the source after injection along the ordinate axis. In this case the velocity distribution of the molecules is taken as a δ -function, the speed ratio determined by the most probable velocity of the background gas is $S = 5$, and the mass ratio is $m_1/m_2 = 10$. The streamlines are given for injection and relaxation in some cylindrical space with the boundary surfaces absorbing the injected gas molecules. This figure readily shows the degradation of the directed motion of the source molecules in the region determined by the relaxation length (in this case $L_r = 20$).

The simulation procedure of relaxation length of the mean kinetic energy of the source molecules to the equilibrium kinetic energy of the background gas is as follows. A reasonably great number of molecular trajectories were simulated by the Monte Carlo method. For each molecule at definite time moments the values of kinetic energy and its distance from the source along the axis were found. After that, for all molecules the

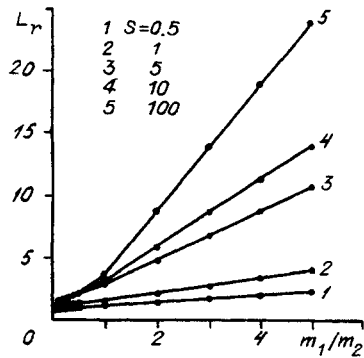


Fig. 3

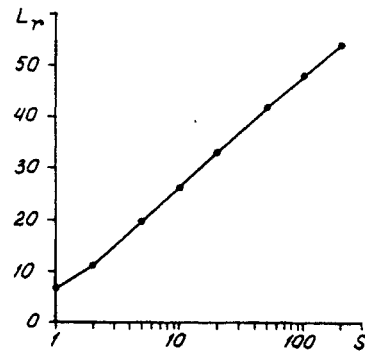


Fig. 4

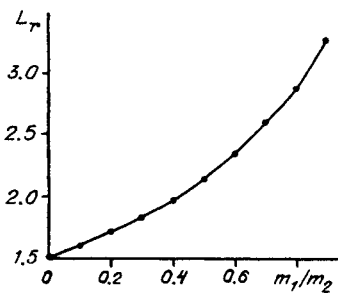


Fig. 5

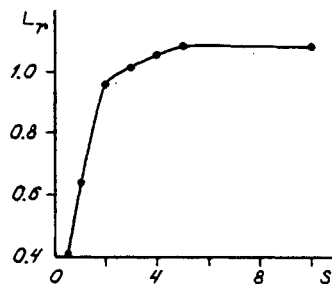


Fig. 6

mean kinetic energy and the mean distance from the source were determined as a function of time. At the instant when the difference between the mean kinetic energy of the background gas molecules and the calculated kinetic energy of the source molecules becomes negligible, the mean distance of the ensemble of molecules from the source is taken as the quantity L_r , which determines the range of the relaxation zone and acts as a characteristic of the kinetic energy relaxation for a given molecular source.

The dependence of L_r on the molecular ratio m_1/m_2 at $S = 1$ is given in Fig. 2. It is seen that the function L_r is linear beginning from the values $m_1/m_2 > 1$ at fixed value of S . The asymptotic behavior of L_r is observed for any value of S (Fig. 3). The dependence of L_r on the velocity ratio S at $m_1/m_2 = 10$ in this region ($m_1/m_2 > 1$) has a logarithmic character (Fig. 4).

For small m_1/m_2 values, the function L_r varies within a narrow range at arbitrary S values. It is pertinent to note some other interesting peculiarities of the behavior of the relaxation length. In the region $m_1/m_2 < 1$, if $S \rightarrow \infty$, L_r tends to a certain limit. The limiting curve is shown in Fig. 5. As an example, Fig. 6 gives the dependence of L_r on S at $m_1/m_2 = 0.1$. At $m_1/m_2 \rightarrow 0$, the limiting value is $L_r \rightarrow 1.5$. We see that $L_r < 1$ for $S < 0.5$. This tendency is obvious, because $L_r = 0$ for $S = 0$.

The change of the fictitious source displacement at $m_1/m_2 \rightarrow 0$ with a change in S is not a manifestation of inertial effects. The fact is, on the average, slow molecules begin their collision process closer to the source. It may be expected that in the injection of a gas with a distribution function different from a δ -function, the gas near the source is colder.

When determining the mean distance characterized by a total loss of the initial momentum, the Monte Carlo simulation of the trajectories of individual molecules were performed until collisions in which the velocity component along the axis changes sign. The average value of this distance over all the molecules was considered as the momentum relaxation length. An interesting feature is that the momentum relaxation length with an error within the statistical spread is equal to the kinetic energy relaxation length of the ensemble of simulated

molecules. An important consequence of this fact is that the dependence for the kinetic energy relaxation length (Figs. 2–6) are valid for the momentum relaxation as well.

An arbitrary source located in the infinite space of a background gas at rest can be a source of spherically symmetric flux governed by the diffusion law. The problem is to find the correct location of the fictitious source. The above analysis answers this question.

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