

KINETICS OF DEGRADATION OF A MOLECULAR BEAM IN A GAS AT REST

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The problem of numerical study of the complete degradation of a stationary molecular beam in a gas at rest consists in the calculation and analysis of the parameter fields of injected molecules formed by translational relaxation from maximum nonequilibrium at an injection point to diffusive drift at the temperature of the background gas. Numerous applied aspects of this problem are referred to different stages of degradation. Beam scattering in the first collisions has been the subject of continuing investigations over many years associated with the creation of molecular-beam equipment, scattering cross-section measurements, and with the determination of intermolecular forces [1, 2]. Most of the publications were devoted to the formation of molecular beams and to the determination of their characteristics [3–5]. Beam degradation determines charge-exchange processes, the possibilities of rejection of electron and ion beams, their purification from neutral particles, and also the methods of creating gas-jet obstructing targets [6–8]. Gas-dynamic separation processes upon injection of a gas mixture and isotopes refer to the stage of substantial degradation of the injected particle flow [9–12]. In gas mixing problems connected with vacuum technologies, the comprehensive characteristic of the process of mixing of an injected gas with a background one is of interest. In particular, to this class of problems one can refer the mixing of molecular and continuum flows under the interaction of a high-altitude rocket engine plume with the ambient atmosphere [13]. Active atmospheric probing by a molecular gas and by electron beams, electron-beam plasma production, and target-surface disintegration by high-energy beams include the final stage of injected beam–background gas interaction.

These processes described by mathematical models have common kinetic phenomena in the transformation of a velocity distribution function of the gas injected into a Maxwellian function corresponding to the state of the ambient gas. In the present paper, we make an attempt to trace the entire process of molecular-beam degradation in the simplest formulation: to investigate the translational relaxation of a unidirectional single-velocity molecular beam of low intensity when the impulsive and thermal actions of the injected molecules on the background gas can be ignored. A similar range of physical problems has been analyzed by Bird [14], Aristov and Shakhov [15], Paklin and Rebrov [16], and Hamel [17]. The paper by Paklin and Rebrov [16] is directly related to the line of research of the present paper.

1. Formulation of the Problem. The direct simulation Monte Carlo method is an effective tool of solving the formulated problem. Since the problem is bounded by the case of a low-intensity molecular beam, intercollisions of injected molecules and their effect on the background gas are not taken into account. The procedure of using the conventional Bird method [18] is modified for the simpler case of a given Maxwellian velocity distribution of background gas molecules. Numerical experiments were performed over a wide range of the masses of injected light ($m_1/m_2 < 1$) and heavy ($m_1/m_2 > 1$) molecules. Here m_1 and m_2 are the molecular masses of the injected and background gases. The beam velocity was varied from zero to values exceeding the mean thermal velocity of the background gas by an order of magnitude. A hard sphere model was employed for description of intermolecular collisions. The parameters of the problem were the mass ratio m_1/m_2 and the speed ratio $S = u_1/V$, where u_1 is the initial velocity of the injected gas and V is the most probable thermal velocity of the background gas.

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The spatial molecular motion was traced in a cylindrical volume at whose boundary the injected molecules were completely absorbed. Injection occurred along the cylinder's axis. The volume dimensions were chosen such that the volume boundaries do not exert a significant effect on the relaxation zone of injected molecules. With allowance for the geometry of the problem, the following cylindrical coordinates were introduced: the x axis coincides with the injection direction, r is the distance to the axis, and φ is the azimuthal angle. As a length unit, we used the length of the free path of a background gas molecule $l = 1/n\sigma\sqrt{2}$ (n is the numerical density and σ is the collisional cross section of the background gas), and the most probable thermal velocity and its temperature were used as the velocity and temperature units, respectively. The trajectories of 10^6 – 10^7 injected molecules were calculated, depending on a concrete formulation of the computational experiment. Based on the accumulated information on the state of injected molecules in the cells, we found their density n , mean mass velocity u , energy E , temperature T , and also the temperature component T_x (energy component E_x) parallel to the cylinder axis and the component T_y (E_y) perpendicular to it. This offered the possibility of analyzing the momentum, energy, and temperature relaxation.

For any mass ratio m_1/m_2 , the statement that at an infinite distance from a source, the mean-mass molecular motion is of a strictly radial character as from a certain fictitious source whose center does not coincide with the position of an injection point is true. The distance L_f from the fictitious source to the injection point is determined by the parameters S and m_1/m_2 . The quantity L_f is the integral characteristic of the relaxation process.

To characterize the relaxation zone, we also used the notion of energy and momentum relaxation lengths. The energy relaxation length L_r was assumed to correspond to a mean distance at which the energy of injected molecules is different from the energy of a background gas by no greater than 1%, and, for the momentum L_i , the relaxation length is defined as a mean distance at which the velocity component of a molecule toward injection changes sign. These quantities are uniquely related to the persistence of the energy and momentum.

2. Analysis of Computational Experiments. To check the algorithm of numerical solution of the formulated problem, in particular, of choosing the volume bounds and the step of a spatial grid, as a test problem, we analyzed the scattering and diffusion of particles produced at the point with zero initial velocity. This corresponds to the case of relaxation and diffusion with absolutely spherical symmetry.

Figure 1a shows the evolution of the velocity distribution function of injected molecules G at distances 0.2, 0.6, and 2.3 of the free-path length for the case $m_1/m_2 = 1$ in comparison with the Maxwellian velocity distribution function corresponding to the energy ("temperature") of the thermal molecular motion at the chosen distances (the solid curve refers to the Maxwellian function, and the dashed curve refers to the distribution function of the injected molecules). Transformation of the injected molecules into Maxwellian ones is mainly completed on three free-path lengths, while the temperature approaches that of the background gas, with a difference of approximately 1% at a distance equal to five free-path lengths (see Fig. 1b). A characteristic feature of the temperature behavior is that the axial temperature component T_x exceeds the radial component T_y .

Figure 2 shows computational results for the case $m_1/m_2 = 1$ and $S = 1$. In this case, the energy ratio of the injected molecules to the background ones is equal to $2/3$. The density, temperature, and energy fields (see Fig. 2a–c, respectively) determine the spatial formation of the relaxation zone. The parameter isolines are shaped like pears. Quantitatively, the relaxation zone can be characterized by the position of the fictitious source at a distance of approximately 1.4 of the free-path length of the background gas from the injection point and by the energy $L_r \approx 2.8$ and momentum $L_i \approx 2.6$ relaxation lengths. Figure 2d gives the evolution of the distribution function along the injection line (the solid curve corresponds to the Maxwellian distribution function, and the dashed line refers to the distribution function of injected molecules). The wake of the initial delta-function disappears at a distance equal approximately to 10 lengths of the free path toward the injection energy. From the back side of the source, the ensemble of injected molecules has a distribution function which is close to a Maxwellian one. The temperature components along the injection line (see Fig. 2e) increase monotonically in the vicinity of the source. Note that at a certain distance, the temperature toward the injection is somewhat higher than that of the background gas. Here and below, the temperature values

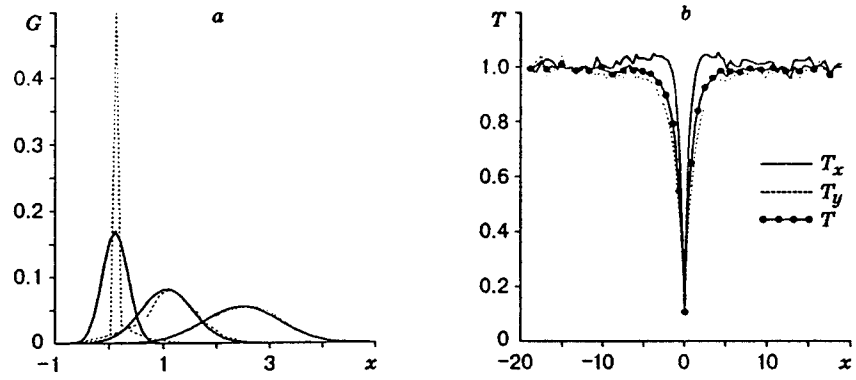


Fig. 1

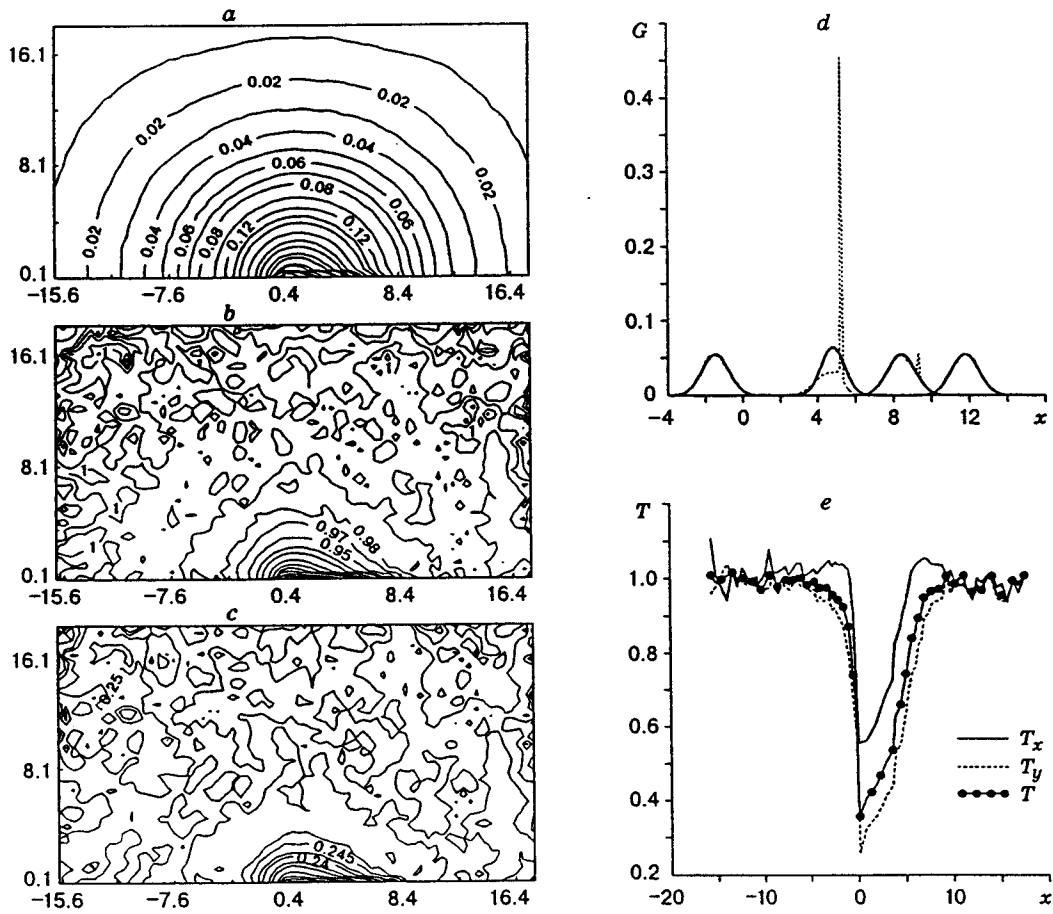


Fig. 2

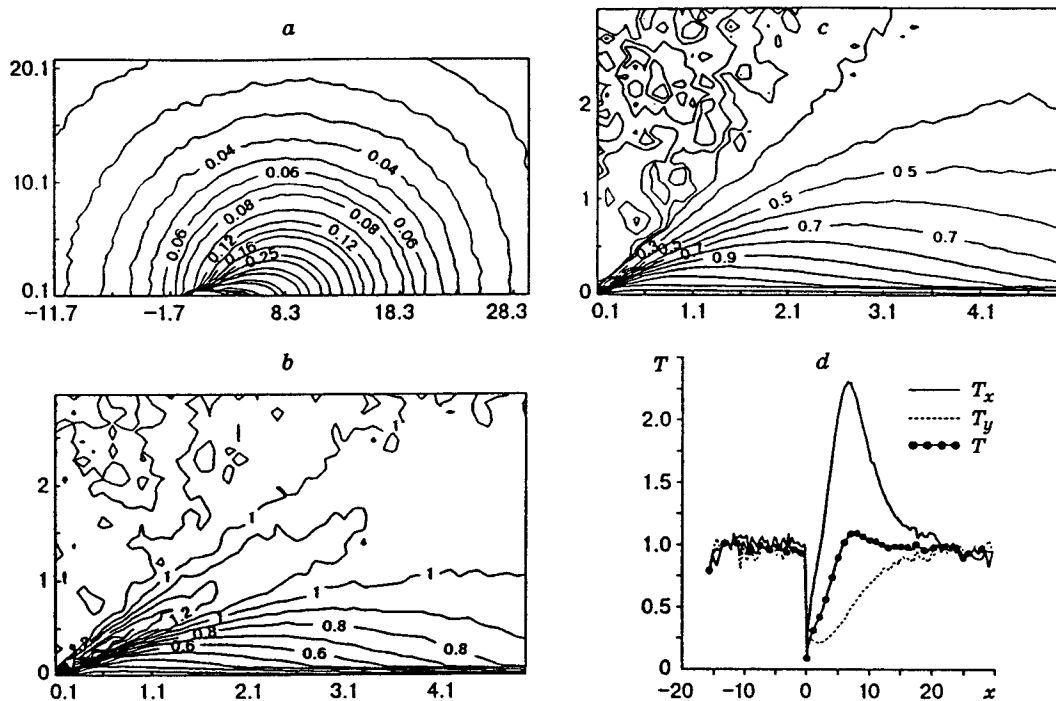


Fig. 3

along the injection line are given for cell sizes along the axis in the vicinity of the source equal to 0.25 of the free-path length of the background gas.

The data obtained on the transformation of the velocity distribution function and of the integral characteristics into Maxwellian ones show the absence of a strong correlation between the distribution function transformation and the energy and momentum relaxation.

In varying m_1/m_2 and S to one side or the other from unity, the relaxation-zone structure does not change significantly. A detailed description of the results obtained is beyond the scope of the present paper, and we shall confine ourselves to the most interesting data for various values of m_1/m_2 and S , giving our attention to analysis of the effect of the injected-gas energy.

Figure 3 shows the density field in the entire computational volume (a), the temperature (b) and energy (c) fields in the initial section of the relaxation zone, and also the variation in the temperature components along the injection line (d) with $S = 1$ and $m_1/m_2 = 10$. The energy of the injected molecules is an order of magnitude greater than in the previous case. The location of the fictitious source is shifted toward the injection direction, and $L_f \approx 8.9$ from the injection point, which corresponds to a strong anisotropy of the relaxation zone. A specific feature of the temperature field is the nonmonotone character of the temperature variation along the normal to the injection line (see Fig. 3b). In the vicinity of a certain surface whose shape is close to an ellipsoid, the injected gas has a very high temperature, with the axis of rotation along the injection direction. As the generatrice, the ellipsoid has major and minor axes equal to five and one free-path lengths, respectively. Within the ellipsoid, a region with a strongly nonequilibrium state is formed. The value of the maximum temperature decreases downstream from the values that are approximately 1.5 times greater than the background gas temperature.

Of course, in the region under consideration, the superposition of the motion of the scattered molecules in the beam and of the molecules moving chaotically in the background gas occurs after the first collisions. Two facts are indicative of a strong effect of the scattered molecules: (a) a monotone decrease in the total energy of the injected gas with distance from the injection point and (b) the presence, on the first 10 free-path lengths, of a maximum of the axial temperature component along the injection direction (T_x in Fig. 3d) with a value that is more than two times higher than the temperature of the ambient gas. This effect can

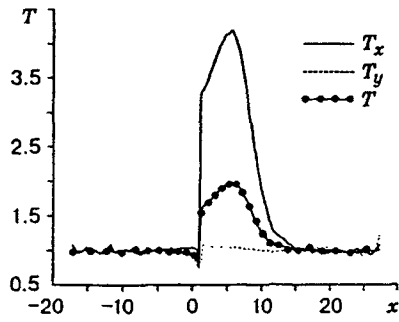


Fig. 4

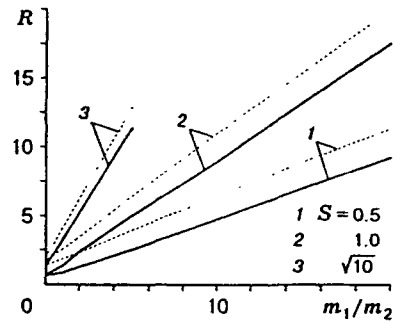


Fig. 5

be obtained only at the expense of molecules that have not yet lost the initial momentum but have already experienced substantial deceleration. The radial temperature component T_y rises monotonically up to the background values. The total (or mean) temperature of the injected gas has a maximum somewhat exceeding the background gas temperature in the vicinity of the fictitious source. The temperature components T_x and T_y behave like those in the shock wave of a monatomic gas on the section of temperature rise. Since the nature of relaxation in both cases is the same, the specific features revealed in the temperature behavior can be called the shock effects of beam degradation.

The data obtained refer to the injection of a heavy gas into a light one. The shock effects becomes significantly pronounced if the injected and background molecules have equal masses, and the energy of injected molecules remains unchanged owing to the increase in their velocity ($S = \sqrt{10}$) (see Fig. 4). The temperature T_x excess the background temperature by more than a factor of 4. It is noteworthy that this excess is close to that occurring in the formation of a shock wave for a monatomic gas with a Mach number close to the selected speed ratio. Variation in the radial temperature component is of a monotone character, and the total temperature has a maximum exceeding approximately twofold the background gas temperature.

If one injects molecules whose mass is tenfold smaller than that of background molecules, at an energy corresponding to the two last cases, a similar shock effect is observed, and the value of the maximum temperature T_x is even higher compared with the preceding case [$(T_x)_{\max} \approx 6$]. But this is much less than the quantity corresponding to gas deceleration at a Mach number close to the value of S . The "softer" shock relaxation effect is due to the fact that the process considered is realized in a mixture of gases with different molecular masses.

Calculations show that if the energy of injected molecules is smaller than that of the background gas molecules, a certain exceeding of the axial temperature component over the background one both for light and heavy molecules is observed only if the energy of the injected molecules approaches the energy of the background gas molecules.

Systematic studies of the degradation kinetics of molecular beams allow one to present sufficiently informative data on their integral characteristics, in particular, to obtain more accurate data compared with [16]. A fictitious source is always in a substantially nonequilibrium relaxation zone. Naturally, the formation of a Maxwellian velocity distribution function is a slower process in comparison with the relaxation of a lower-order momentum distribution function. The characteristic dimensions of relaxation zones grow with increasing ratio between the molecular masses m_1 and m_2 . With $m_1 > m_2$, the relaxation zone is elongated toward the injection direction. For $m_1 < m_2$, a decrease in the mass ratio makes the relaxation zone more spherically symmetric.

Figure 5 shows the distances from the injection point to the fictitious source (solid curves) and the momentum relaxation length (dashed curves) for $S = 0.5, 1, \text{ and } \sqrt{10}$ within the range of mass ratios m_1/m_2 0.1–20. The data obtained support the results of [16]. It turned out that the momentum relaxation length correlates with the position of the fictitious source. As one should expect, for all values of S , the position of the fictitious source and the boundaries of the complete momentum relaxation are shifted toward the injection

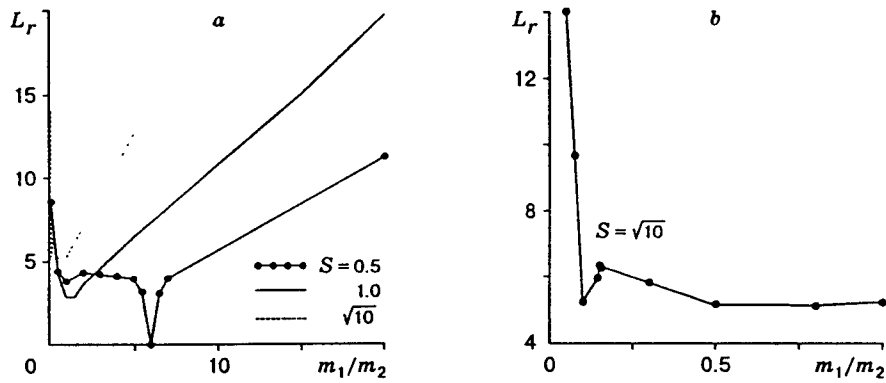


Fig. 6

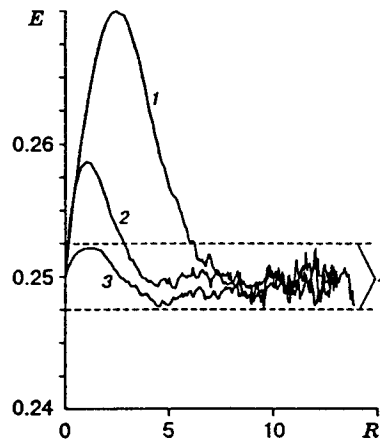


Fig. 7

relaxation even for $m_1/m_2 \ll 1$.

The energy dependence of the relaxation length $L_r = G(m_1/m_2, S)$ is of a complicated character (see Fig. 6a). For $m_1/m_2 \rightarrow 0$, $m_1/m_2 \rightarrow \infty$ and a fixed S , the value of L_r increases, and two minima are observed. With $S < 1$, one minimum is in the vicinity of the point $m_1 = m_2$, which corresponds to a faster relaxation, with molecular masses being equal, and the other is in the vicinity of the point corresponding to equal energies of the injected and background molecules. For $S = 0.5$, the minimum of L_r appeared to be pronounced, with equal energies. For the adopted computational boundary of the relaxation energy (the difference of the background gas energy amounts to 1%), $L_r \rightarrow 0$. For $S > 1$, the minimum in the vicinity of the point with equal masses is preserved. The position of the second minimum depends on the specific features of the relaxation of light molecules at high injection velocities. Figure 6b shows separately the variation in L_r for $S = \sqrt{10}$. The minimum value of L_r amounts to five to six free-path lengths, and the second minimum occurs at an energy of the injected molecules smaller than the energy of the background gas molecules.

To account for the specific features revealed, we calculated the variation in the energy of injected molecules in the initial period of relaxation for various masses of the molecules whose energy equals that of the background gas molecules. Curve 1 in Fig. 7 corresponds to the case $m_1/m_2 = 0.15$ and $S = \sqrt{10}$, curve 2 refers to $m_1/m_2 = 1.5$ and $S = 1$, curve 3 refers to $m_1/m_2 = 6$ and $S = 0.5$, and curves 4 bound the region in which the energy deviation from the background value is less than 1%. The relaxation of light molecules turned out to be accompanied by a marked initial increase in energy at a distance equal to the first five free-path lengths. For example, for $m_1/m_2 = 0.15$, the energy exceeds the initial one by approximately 8%. It follows that, for $S > 1$, the position of the second minimum can be not coincident with the point of energy equality. The increase in the energy of heavy molecules decreases considerably with increasing mass

of the injected molecules. With $m_1/m_2 > 6$, the increase is less than 1%, i.e., the relaxation of mean-energy heavy molecules, which, in practice, is not disturbed by collisions, can be considered completed at distances from the source which are smaller than one free-path length.

The computations made it possible to establish that, with energies of the injected and background molecules being equal, the energy-relaxation length is not the spatial characteristic of the relaxation zone, because the Maxwellian velocity distribution function of the molecules has no unambiguous correlation with the relaxation energy. However large in dimensions, the relaxation zone of the velocity distribution function of the molecules can be completely isothermal beyond the first five free-path lengths, depending on m_1/m_2 and S .

Conclusion. Based on a direct simulation, comprehensive and systematic studies of the degradation kinetics of a molecular beam at rest made it possible to reveal the qualitative and quantitative relaxation characteristics of the molecular beam to thermal equilibrium with the background gas within the ranges of mass ratios of the injected and background gases 0.1–20 and within velocity ratios of the injection $0.5-\sqrt{10}$ for model molecules as hard spheres. The conclusions on the qualitative character of degradation are valid for a wider spectrum of parameters as well. As is established, at an energy of the injected molecules exceeding that of the background gas, during relaxation, a shock effect, i.e., the exceeding of the thermal energy of the injected gas over that of the background gas, is observed. Having been evaluated by analogy with supersonic-flow deceleration, the shock effect is the stronger, the closer the molecules of the injected and background gases in their masses. An initial increase in the energy of the injected molecules that is more considerable for light molecules has been discovered. The dependence of the energy relaxation length on the ratio of the masses and initial velocities of injected molecules has been established.

The data obtained allow us to estimate the dimensions of the region of nonequilibrium mixing of injected and background gases with small values of the intensity of molecular flow in the beam.

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