ESCAPE INTO A VACUUM OF A BINARY GAS MIXTURE WITH
COMPONENTS OF CONSIDERABLY DIFFERENT MOLECULAR WEIGHTS

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The trajectory method is generalized to the case of the escape into a vacuum of a binary gas mixture with molecules of considerably different masses and sizes, with allowance for the initial nonuniformity of the distribution of the heavy component in velocity space.

In an analysis of the problem of supersonic flow of a gas mixture of components with considerably different molecular weights, by analyzing the Boltzmann equations one can indentify two characteristic zones and construct mathematical models of the flow in each of them.

The model proposed here enables one to allow for the velocity spread of the heavy component and is, in this sense, a generalization of the dynamics of multiphase systems based on the trajectory model [1]. The transport of SF_6 molecules by N_2 carrier gas is calculated below as an example. Calculated results are given for different values of the escape parameters.

Such an approach obviously can be used to solve the problem of the transport of clusters, which are formed in supersonic nozzles and jets, by the light (carrier) component. This is related primarily to the fact that small clusters cannot be treated as particles of an impurity phase, applying directly to the calculation of their motion the methods of the mechanics of multiphase media, based on the hypothesis [2] of interpenetration of continua, of which only the carrier gas has an intrinsic pressure, since the random motion of clusters cannot be ignored in an analysis of a "gas" of small clusters. During expansion in a nozzle or a supersonic jet, however, the drop in the density of the escaping gas mixture means that it becomes possible to ignore the interaction between particles of the disperse phase and, after some generalization, to use the methods of calculation of multiphase media.

An analysis of the flow of a binary mixture in a nozzle or jet enables one to identify the following characteristic regions of flow.

1. A zone in which one cannot ignore collisions between heavy particles (molecules) and, in this connection, one cannot consider the "gas" of particles to be a medium without pressure. To calculate the flow of such a mixture, one can use the ideal of an equivalent gas with an effective molecular mass and an effecitve adiabatic index, as is usually assumed for a binary gas mixture.

2. A zone in which the motion of the heavy component can be treated as the motion of a collisionless mixture; here one must remember, however, that the initial conditions for the particle parameters are the conditions determined by flow in the preceding zone.

In this case, in addition to the mean hydrodynamic velocity, the particles will possess a velocity spread about the mean value. Whereas in calculating the parameters of the motion of heterogeneous media one can, because of the enormous difference in masses, neglect the departure of the velocities of heavy particles from the mean value, in the present case this neglect may result in considerable errors in obtaining the spatial distributions of the particles.

Such a division has a purely arbitrary nature, of course, since here we ignore the existence of a transition zone, in which neither of the proposed approximations may be used. The question of the possibility of calculating the parameters in this zone will be considered
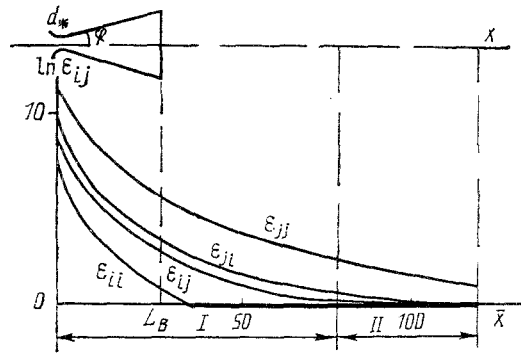
Fig. 1. Variation of the dimensionless parameters to the collision integrals for molecules of the light (ε_{gg}) and heavy (ε_{pp}) gases and for collisions between them (ε_{pg}, ε_{gp}) along the axis of symmetry of the jet: I, II) first and second calculation zones (ε_{ij}, $i = p$, g; $j = p$, g).

below. We note that this division has more a relative nature and is founded on empirical considerations. In this connection, it would be desirable to obtain more rigorous estimates of the possibility of using the proposed approach and fairly well-founded equations for the macroscopic parameters of the mixture. The kinetic approach to describing the motion of a heterogeneous mixture, developed in [3], seems the most promising for achieving this aim. In accordance with this approach, a Boltzmann equation with interphase collision integrals is written for each component of the mixture. After these equations are made dimensionless, it becomes possible to isolate the dimensionless parameters that determine the form of the equations describing the flow in each of the aforementioned zones.

1. Estimation of the Parameters of the Kinetic Equations

Let us consider the system of Boltzmann equations for a mixture of heavy and light components,

$$Df_g = \varepsilon_{gg} I_{gg} + \varepsilon_{gp} I_{gp}, \quad Df_p = \varepsilon_{pp} I_{pp} + \varepsilon_{pg} I_{pg}, \tag{1}$$

where f_g and f_p are the distribution functions for the light and heavy gases, respectively. The dimensionless parameters in the collision integrals are (see [3])

$$\varepsilon_{gg} = \frac{L}{l_{gg}} = \frac{L\sigma_{gg} n_g}{u_g} \sqrt{\frac{kT_g}{m_g}}, \quad \varepsilon_{gp} = \frac{L}{l_{gp}} = \frac{L\sigma_{gp} n_p}{u_g} \sqrt{\frac{kT_g}{m_g}},$$

$$\varepsilon_{pp} = \frac{L}{l_{pp}} = \frac{L\sigma_{pp} n_p}{u_p} \sqrt{\frac{kT_g}{m_p}}, \tag{2}$$

$$\varepsilon_{pg} = \frac{L}{l_{pg}} = \frac{L\sigma_{gp} n_g}{u_p \varepsilon_m} \sqrt{\frac{kT_g}{m_p}}, \quad \varepsilon_m = \sqrt{\frac{m_g}{m_p}},$$

where $\sigma_{gg} = \pi d_g^2$; $\sigma_{gp} = \frac{\pi}{4}(d_g + dp)^2$; $\sigma_{pp} = \pi d_p^2$ are the scattering cross sections; m_g, m_p, d_g, and d_p are the masses and radii of molecules of the carrier gas and of the heavy molecules, respectively; k is the Boltzmann constant; L is the characteristic size for the problem; T_g, T_p, n_g, and n_p are the characteristic kinetic energies and number densities of the carrier and heavy gases; u_g and u_p are the characteristic velocities of the components. We note that until the transition to the equations for the macroscopic parameters has been made, we cannot talk about such macroscopic characteristics as the temperature, the hydrodynamic velocity of the medium, etc. In this connection, we shall understand the characteristic values of the parameters to be the values of the mean velocity and the mean energy of the random motion. In analyzing Eqs. (1) with respect to the parameters (2), we can distinguish the following cases:

1)
$$\varepsilon_{gg} \gg 1, \ \varepsilon_{pp} \gg 1, \ \varepsilon_{gp} \gg 1, \ \varepsilon_{pg} \gg 1.$$

This case corresponds to the flow of a binary, one-temperature, one-velocity mixture, since the presence of a large parameter on the right sides of all the equations in system (1) indicates that global Maxwellian equilibrium is established at times much shorter than the gas-dynamic time [4]. We may thus talk about the motion of a one-temperature, one-velocity medium, for which we may introduce the concept of an equivalent gas with an effective molecular weight on an effective adiabatic index. This corresponds to the first zone of calculation mentioned above:

2)
$$\varepsilon_{gg} \gg 1, \ \varepsilon_{pp} \gg 1, \ \varepsilon_{gp} \gg 1, \ \varepsilon_{pg} \ll 1.$$

A one-velocity, two-temperature flow regime occurs in such a situation. The motion of the mixture may then be described by the energy continuity equations for each of the components and by a general equation of momentum transport. In the present work we shall ignore the existence of a region with such a relationship of dimensionless parameters.

3)
$$\varepsilon_{gg} \gg 1, \ \varepsilon_{pp} \leqslant 1, \ \varepsilon_{gp} > 1.$$

This combination of parameters corresponds to the transitional regime, in which the collisional and convective parts of the Boltzmann equation for the heavy component become equal in order of magnitude. Calculating in this zone presents the greatest difficulties, but this zone is often negligible in zize, according to estimates. Otherwise, one can, using the moment method, for example, obtain equations for the macroscopic parameters of the components. This derivation is not given here because the transition zone is fairly small in the problem under consideration.

4)
$$\varepsilon_{gg} \gg 1, \ \varepsilon_{pp} \ll 1, \ \varepsilon_{gp} \sim 1, \ \varepsilon_{pg} \sim 1.$$

In the latter case, because $\varepsilon_{pp} \ll 1$, we can ignore collisions between heavy molecules, and the collision integral for molecules of the light gas becomes the leading term determining the collisional part of the Boltzmann equation for the heavy component. Because $\varepsilon_{pg} \approx 1$, the collisional and convective parts have the same order of magnitude. Equations for the macroscopic parameters of the heavy gas may be derived using the moment method. This case obviously corresponds to the second calculation zone indicated above. It must be noted, however, that after the equations for the macroscopic parameters have been obtained from the Boltzmann equation by the moment method, a problem arises in connection with the solution of these equations, since in the initial cross section of this calculation zone the velocity distribution function of the heavy component is not deltoid, which prevents the direct use of the trajectory method that is widely used to calculate a collisionless mixture. One possible way of solving this problem is given below:

5)
$$\varepsilon_{gg} \gg 1, \ \varepsilon_{pp} \ll 1, \ \varepsilon_{gp} \ll 1, \ \varepsilon_{pg} \ll 1.$$

Case 5) corresponds to free dispersal of the heavy molecules without interacting with each other or with the carrier component. In concluding this section, we note that we have considered only conditions under which $\varepsilon_{gg} \gg 1$. Here the latter case may not occur in pratice.

2. Conversion to Macroscopic Parameters

As noted above, the equations for the macroscopic parameters of the components, which correspond to the first calculation zone, are the equations of motion of an equivalent gas with effective parameters, so no problems arise in connection with calculating the parameters of motion of such a gas. Matters are different in the second calculation zone. Let us consider this problem in more detail. We start with an examination of the trajectory model, which is widely used to calculate flows of mulitphase media, but which is well-founded at present only at the phenomenological level, being based on arguments of an empirical order. If we consider the normalized distribution function of the heavy molecules, then for this model it is $f_p = n_p(r_p, t)\delta(\mathbf{v}_p - \mathbf{u}_v)$, i.e., we assume that at each point of space there is no spread in the velocities of the particles owing to their fairly large mass. In the initial cross section of the calculation zone we now subdivide all of coordinate space into regions
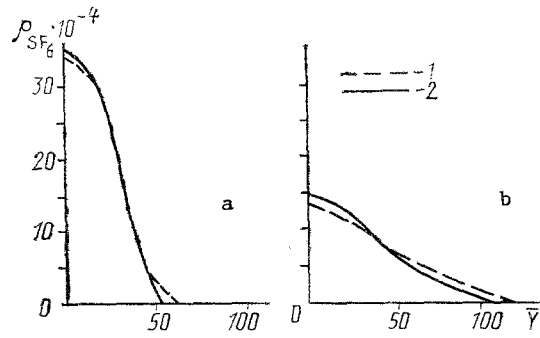
Fig. 2. Distributions of mass density of the heavy
component (SF_6 molecules) in cross sections of the
jet at the following distances from the critical
cross section of the nozzle: a) X = 0.08 m; b) 0.120 m;
1) calculations with (N_v = 13) and 2) without (N_v =
1) allowance for the initial velocity nonuniformity
of the heavy component ($\overline{Y}$ = Y/d$_*$, $\overline{X}$ = X/d$_*$). ρ_{SF_6},
kg/m^3.

$\Omega_r = \{R_p, R_p + \Delta R_p\}$, with $\Delta R_p \to 0$. We juxtapose each region Ω_r to a characteristic function,

$$X_r = 1 \text{ for } r_p \in \Omega_r,$$

$$X_r = 0 \text{ for } r_p \notin \Omega_r. \tag{3}$$

Using the fact that $\Delta R_p \to 0$, we may approximate the function f_p as precisely as derived by
the sum $\sum_r^\infty N_p X_r \delta(\bar{r}_p - \bar{R}_p)$ where N_p is the number density of particles whose coordinates lie
inside region Ω_r. In accordance with this method of subdivision, we can treat the initial set
of particles of the heavy component as a mixture of gases that differ only in their positions
in the initial calculation cross section. if we now formally write the Boltzmann equation
for such gas,

$$D(\delta(\bar{v}_p - \bar{u}_p)N_p) = \left[\frac{\partial(\delta(\bar{v}_p - \bar{u}_p)N_p)}{\partial t}\right]_{coll}, \tag{4}$$

where u_p is the mean velocity of the ensemble of particles from region Ω_r and $\bar{v}_p$ is the veloc-
ity of an individual particle, then because the particles do not collide with each other,
the right side of Eq. (4) determines only the collisions with molecules of the light (carrier)
gas. Using the component method [4], it is easy to show that after integrating Eq. (4) over
velocity space and the coordinates with weights $\varphi = 1$, r, $\bar{v}_p$, we obtain the equations

$$\frac{dN_p}{dt} = 0, \tag{5}$$

$$\frac{dR_p}{dt} = u_p, \tag{6}$$

$$\frac{du_p}{dt} = -F_{pg}. \tag{7}$$

In integrating Eq. (4), we use the fact that the relative flow of the light component occurs
in the free-molecule regime; the collision integral for heavy molecules colliding with light
ones is converted into the force of interaction between the components,

$$F_{pg} = C_D \frac{\pi d_p^2 \rho_g (u_p - u_g) |u_p - u_g|}{8 m_p},$$

where C_D is the coefficient of aerodynamic drag of a praticle (molecule), which may be determined analytically [5]. Equations (6)-(7) thus correspond fully to the equations of a test particle in the trajectory model, while Eq. (5) describes the conservation of particle number along its trajectory. If we now return to the problem of calculating the parameters in the second calculation zone, then the velocity distribution function of molecules of the heavy component in the initial cross section is not deltoid, as noted earlier, which hinders the use of the above-described method. If we now extend the discussion of this model to the case of velocity nonuniformity of the heavy molecules at a fixed point of physical space, however, then the phase space of velocities and coordinates can be subdivided into regions $\Omega = \Omega_r + \Omega_v$, with $\Omega_v = \{u_p, u_p + \Delta v\}$, and we can introduce the corresponding characteristic functions χ_v by analogy with (3). it is then easy, by manipulations analogous to the foregoing, to obtain equations analogous to (5)-(7).

This actually means that after subdividing the heavy gas in physical space into individual fractions Ω_r, lying at every fixed point of the initial cross section, we subdivide each of these fractions into fractions Ω_v in accordance with the particle velocity distribution. We use the usual method of calculating multiphase flows, calculating the parameters of the carrier gas using a Godunov difference scheme, and integrating Eq. (7) along the trajectories of test particles [1].

3. Numerical Realization and Calculation Results

The results of a calculation of the transport of SF_6 molecules by nitrogen in a conical nozzle during escape into a vacuum are given below as an example. In the first calculation zone, where the flow of the mixture may be described by an equivalent gas, a steady-state Godunov analog — the Ivanov—Kraiko scheme [6] — is used to calculate the parameters. To calculate the flow parameters in the second zone, the same scheme is used for the carrier phase, while the parameters of the heavy gas are obtained by integrating Eq. (7) along the trajectories. Here the force interaction between components [1] is taken into account at each half-step, which is chosen from the conditions of stability in calculating the parameters of the carrier gas. To satisfy Eq. (6), the constancy of the flow rate n_p^Ω along the streamline of each ensemble, discussed above, is taken into account in calculating the parameters. The calculation was made for the following parameters (see Fig. 1): diameter of critcal cross section $d_* = 1 \cdot 10^{-3}$ m, half-aperture angle of nozzle $= 17°$, pressure in receiver $P_0 = 1.5 \cdot 10^5$ N/m², nozzle length $L_B = 0.03$ m, length of entire calculation zone $L_R = 0.12$ m, volumetric fraction of heavy component $Z = 0.05$, and $\varepsilon_m = 0.45$. The number of calculating cells was chosen to be $N = 30$ for the carrier gas and the number of subdivisions of physical space for the heavy gas was $N_r = 30$. The program was written in Fortran-IV, the calculations were made on an ES-1045 computer, and the calculation time was bout 20 min with $N_v = 1$ and about 60 min with $N_v = 13$.

In Fig. 1 the variation of the dimensionless parameters of Eqs. (1) along the flow axis is shown, and calculation zones I and II are shown in accordance with the estimates (3)-(6). The distribution of the concentration of the heavy component SF_6 perpendicular to the flow axis in two calculation cross sections is shown in Fig. 2. Here we give the results of calculations for different numbers N_v of subdivisions into ensembles N_p in velocity space. From these results it follows that allowance for velocity nonuniformity at the calculation points of the initial cross section leads to a slight change in the concentration profile of the heavy SF_6 molecules in the control cross section. Here it is sufficient to limit the number of subdivisions into ensembles N_p in velocities to $N_v = 13$, since further subdivision results in no significant change in the concentration profile. The total number of trajectories of heavy particles was $N_{rv} = N_r N_v = 390$ in this case.

In conclusion, we note that the method developed is a generalization of the trajectory method to the case of allowance for initial nonuniformity of the distribution in velocity space. Characteristic zones of flow are distinguished, among which the region of applicablity of the trajectory method [1] is designated, including that for two-phase flows.

NOTATION

I, ε, collision integrals and dimensionless parameter in them; f, distribution function; σ, scattering cross section; m, ρ, mass and mass density; d, diameter; T, n, characteristic kinetic energy and number density; u_*, characteristic velocity; k, Boltzmann constant; $\bar{u}_p$, mean velocity vector of the ensemble of heavy gas molecules from region Ω_r; $\bar{V}_p$, mean velocity vector of an individual heavy gas molecule; C_D, drag coefficient of a heavy molecule in relative flow of the light gas over it; P_0, pressure in receiver; L_B, L_R, lengths of nozzle and calculation zone; φ, half-aperture angle of nozzle cone; Z, volumetric fraction of heavy component; N_r, N_v, numbers of subdivisions of physical space and with respect to velocity. Subscripts denote the following parameters: g, light (carrier) gas; p, heavy gas; *, in the critical cross section of the nozzle.

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