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NUMERICAL SIMULATION OF VIBRATIONAL RELAXATION PROCESSES IN UNSTEADY GAS JETS

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The formation of supersonic jet when an axisymmetric or planar nozzle is turned on has been the subject of a considerable number of experimental and theoretical studies, mainly in the ten years [1-4]. At the same time, the processes involved in such flows is not as well as understood as are steady-state jets. In particular, relaxation phenomena in two-dimensional unsteady jets, which can substantially affect the gasdynamic structure of the flow, have not been investigated well.

1. Qualitative Laws. The process of starting a supersonic jet can be illustrated with the example of a simple laboratory model, in which at the initial time gas fills a high-pressure chamber, separated from a low-pressure chamber by a diaphragm. When the diaphragm ruptures, gas begins to flow through the nozzle into the low-pressure region, which is filled with a foreign gas. The outflowing gas acts as sort of piston, which produces a shock wave inside the foreign gas. At the same time, in the foreign gas a rarefaction wave forms with its center at the nozzle inlet and a constant flow is established in a time of the order of $t_* \sim r_*/c_*$ (r_* and c_* are the radius and velocity of sound in the nozzle throat).

Initially the front of the outflowing gas moves according to the linear law $x \sim t$, i.e., as if this gas were flowing into a vacuum. Clearly, there should be a characteristic time t_0 at which the flooded space begins to have an effect and the dimensions of the region occupied by the flow begin to exceed r_* many times. No characteristic quantities with the dimension of length remain in the problem, which has a self-similar solution (when flow anisotropy is ignored).

$$x \sim t^{2/(n+2)}$$

($n = 1$ and 2 for a slotted and a cylindrical nozzle, respectively).

Estimates for the laws of motion of a strong explosion in the one-dimensional approximation were made in [4], using the theory of a thin shock layer; the time t_0 characterizing the change of flow modes is given in [5].

At times $t >> t_0$ the counter pressure begins to play an increasing role, the mass of gas beyond the contact boundary increases, and finally a secondary shock wave, matching the pressure in the outflowing gas to the ambient pressure, forms in the working gas. This wave, propagating upward along the flow with velocities slower than the velocity of sound, gradually drifts from the section where it is formed near the nozzle to its steady-state position [6]

$$x_{sl} \simeq 1{,}5(p_0/p_\infty)^{1/n} r_*,$$

where p_0 and p_∞ are the stagnation pressures of the gas and the flooded space. Almost simultaneously, a shock-wave structure characteristic of a steady underexpanded jet is formed in the region adjacent to the nozzle exit.

All of the above pertains to the formation of an equilibrium jet. At the same time, however, against the background of gasdynamic processes vibrational relaxation processes occur with characteristic times comparable to the rise times. The disequilibrium effects, in turn, affect the gasdynamic characteristics of the flow field

2. Basic Equations. The process of formation of a relaxing jet is described by the system of equations

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$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0,$$
$$\frac{\partial(\rho u)}{\partial t} + \operatorname{div}(\rho u \mathbf{v}) + \frac{\partial p}{\partial x} = 0, \quad \frac{\partial(\rho w)}{\partial t} + \operatorname{div}(\rho w \mathbf{v}) + \frac{\partial p}{\partial y} = 0,$$
$$\frac{\partial(\rho e)}{\partial t} + \operatorname{div}((\rho e + p)\mathbf{v}) = 0,$$
$$\frac{de_i^{(\omega)}}{dt} = F_i(\xi_s, T, p, e_j^{(\omega)}), \tag{2.1}$$

where ρ is the gas density; p is the gas pressure; T is the temperature; e is the total energy of a unit mass of the gas; u and w are the components of the velocity **V** along the x and y axes (here and below the variable x is directed along the axis and y, orthogonally to the axis of the flow); ξ_s is the concentration of the s component of the mixture; and $e_i^{(v)}$ is the energy of the i-th vibrational mode.

The relaxation equations describe the variation the vibrational mode energies, with the function $F_i(\xi_s, T, p, e_j^{(v)})$ characterizing the relation between the i-th mode and all the others. The most important relaxation channels in the gas mixture considered (CO_2, N_2, and H_2O) are:

$$CO_2(010) + M_i \rightleftarrows CO_2(000) + M_i,$$
$$N_2(1) + M_i \rightleftarrows N_2 + M_i,$$
$$CO_2(100) + M_i \rightleftarrows CO_2(020) + M_i,$$
$$CO_2(001) + M_i \rightleftarrows CO_2(030,110) + M_i,$$
$$N_2(1) + CO_2(000) \rightleftarrows N_2 + CO_2(001).$$

Here $M_i = CO_2$, N_2, H_2O. The relaxation equations were described in the harmonic oscillator approximation [7] on the assumption that each vibrational mode i had a Boltzmann distribution with vibrational temperature T_i (in particular, T_1, T_2, T_3 are the vibrational temperatures of the symmetric, deformation, and antisymmetric modes, respectively, of CO_2 and T_4 is the vibrational temperature of N_2).

3. Method of Calculation. The numerical scheme for solving the resulting system of equations was chosen on the basis of the method of large particles [[8]. Within the framework of this method the initial system of equations (2.1) is split according to physical processes. The "still terms," describing the vibrational relaxation itself, now appear only in the system of the first (Eulerian) stage and can be integrated over each times step. At the same time the gas parameters at the boundaries of the computing cells were calculated by the "decay of explosion" scheme [9]; this made it possible to correctly describe the gradient terms in the regions where the flow turns, in particular at the nozzle edge.

Following [8], we split the system of Eqs. (2.1) into two subsidiary systems. Then for the Eulerian stage we obtain

$$\frac{\partial \rho}{\partial t} = 0, \; \rho \frac{\partial e}{\partial t} + \operatorname{div}(p\mathbf{v}) = 0,$$
$$\rho \frac{\partial u}{\partial t} - \frac{\partial p}{\partial x} = 0, \; \rho \frac{\partial w}{\partial t} + \frac{\partial p}{\partial y} = 0,$$
$$\frac{\partial e_i^{(\omega)}}{\partial t} = F_i(\xi_s, T, p, e_j^{(\omega)}),$$

and for the Lagrangian we have

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0,$$
$$\frac{\partial \rho u}{\partial t} + \operatorname{div}(\rho u \mathbf{v}) = 0, \quad \frac{\partial \rho w}{\partial t} - \operatorname{div}(\rho w \mathbf{v}) = 0,$$
$$\frac{\partial \rho e}{\partial t} + \operatorname{div}(\rho e \mathbf{v}) = 0, \quad \frac{\partial \rho e_i^{(\omega)}}{\partial t} + \operatorname{div}(\rho e_i^{(\omega)} \mathbf{v}) = 0.$$

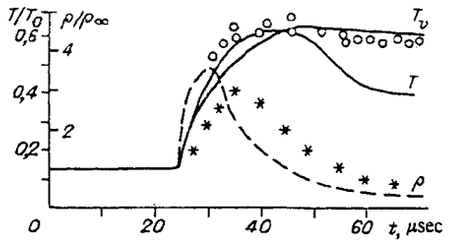

Fig. 1

The relaxation equations contain source terms of the form $p\left(\frac{e_i^{(v)0} - e_i^{(v)}}{\tau_i} \ldots\right)$, where $e_i^{(v)0}$ is the equilibrium value of the energy and τ_i is the relaxation time of the i-th vibrational mode. These terms have a deleterious effect on the stability of the system as a whole, making it stiff [10]. An implicitly numerical scheme is generally used to integrate such stiff systems and as a result unconditional stability of the calculation is ensured. Unfortunately, the development of completely implicit schemes for the problem of multidimensional hydrogasdynamics involves considerably technical difficulties. The different approach used here [11] makes it possible to overcome those difficulties. With this approach integration of stiff terms and equations is put into a separate stage, in which all gasdynamic parameters are assumed to be constant. As mentioned above, in the large particles method the initial system of equations is split according to physical processes. Indeed, the "stiff terms" describing the vibrational relaxation itself are now contained only in the system of the first (Eulerian) stage and can be integrated over each time step. We can write each relaxation equation as

$$\frac{de_i^{(v)}}{dt} = a_i - b_i e_i^{(v)}, \tag{3.1}$$

having grouped terms that do contain $e_i^{(v)}$ and those that do not. The coefficients a_i and b_i are unwieldy expressions, which are given in [5]. Assuming that those coefficients are constant on each integration step, we solve system (3.1) and obtain

$$e_i^{(v),\,t+\Delta t} = \frac{a_i}{b_i} + \left(e_i^{(v),\,t} - \frac{a_i}{b_i}\right)\exp(-b_i\Delta t),$$

where Δt is the integration step of the relaxation equation; $e_i^{(v),\,t}$, $e_i^{(v),\,t+\Delta t}$ is the vibrational energy of mode i at the beginning and end of the integration step.

The finite-difference approximation of all the other terms on a computational grid with (Δx_i, Δu_i) cells is standard [8], and we will not dwell on it. The range of integration is divided into three parts, modeling the high-pressure chamber, low-pressure chamber, and nozzle. In the cylindrical (Cartesian) coordinate system each region was covered with cells having sides of Δx_i and Δy_i (i and j are the cell numbers). The regions adjacent to the nozzle on either size were covered with a grid of constant spacing. Starting from a number N_x^* and N_y^* (k = 1, 2 for the high-pressure and low-pressure chambers, respectively, the cell sides increased according to the law $\varepsilon^{-N^k_{x(y)}+n+1}$ ($n = i,j$ and $\varepsilon \geq 1$ [12]).

The boundary conditions were given as follows: the solid walls (nozzle and wall separating the computational regions) are sealed while the conditions at the outer walls of a computational region are the same as in the corresponding chamber. At the same time, the program also provided for boundary conditions so that the gas counterflow and wake could be described.

The asymptotic approximation of the values of the flow parameters calculated by the above procedure to the values calculated by the method used to calculated a steady jet [13], generalized to the case of vibrational-nonequilibrium flows, was used to check that a steady flow had been established.

The computational scheme described above was implemented in a program used for numerous computations for the following range of parameters: the off-design factor, i.e., the ratio of the pressure at the nozzle exit to the pressure in the flooded space varied from 10 to 10^8, and the Mach number of the jet at the exit varied from 0.7 to 10. Moreover, during the calculations we varied the geometry of the nozzle (and, hence, of the flow), the concentrations of the components in the mixture, the initial temperatures in the high-pressure and low-pressure chambers, the nozzle throat diameter, etc.

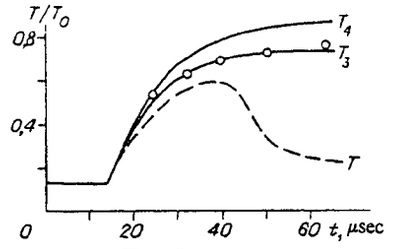

Fig. 2

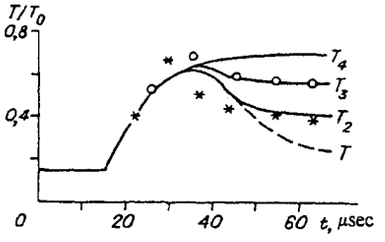

Fig. 3

Unfortunately, the capability of the program described above was limited seriously by the insufficient memory and speed of the computer used. In practice, therefore, all of the results reported below pertain to a region no more than 40-50 calibers in size adjacent to the nozzle.

4. Comparison with Experiment. The results of the numerical computation were compared with the experimental data obtained on a setup combining a shock tube of diameter 50 mm with a flat vacuum chamber in which a two-dimensional gas jet was bounded by walls at a distance L = 45 mm [5]. Gas heated by the reflected shock wave flowed out through a slit of half-width $h_* = 1$ mm. The low-pressure chamber of the shock tube and the vacuum chamber were filled with the gas under study to a pressure $p_\infty = 1.3 \cdot 10^3$-$2.6 \cdot 10^4$ Pa. The pressure of the driver gas (He) was $2 \cdot 10^{-6} - 5 \cdot 10^6$ Pa. The equilibrium parameters of the gas beyond the reflected shock wave, i.e., the parameters of the drag of the outflowing jet, varied over the ranges $T_0 = 1500$-2500 K and $p_0 = 10^{-6}$-$6 \cdot 10^6$ Pa. The diagnostics of a pulsed jet was done by means of multichannel emission and absorption spectroscopy in the visible [2] and infrared regions.

The experimental results for the steady stage of jet flow were compared with the calculations for steady jets and the asymptotic form of unsteady calculations. The results obtained by various methods were found to be in good agreement. The greatest discrepancy between the steady calculation and the experiment is for the vibrational temperatures of CO_2 in a mixture of CO_2, N_2, and H_2O. The explanation for this is that the parameters at the observation point do not manage to reach steady-state values during the experiment.

The characteristics of the flow in the unsteady stage of jet flow, which were determined in the experiments in the form of time dependences of the density and the vibrational temperatures at fixed points on the axis of the flow, were compared with the results of calculations in the same coordinates.

Figure 1 shows the variation of the density ρ, vibrational temperature T_v, and translational T on the axis of the CO_2 jet at distances $x = 28\ h_*$ from the nozzle exit: the points represent the averaged data from experiments with $T_0 = 2000$-2400 K, $p_0 = 2 \cdot 10^6$-$3.5 \cdot 10^6$ Pa, $p_\infty = 3 \cdot 10^3$-10^4 Pa, and the curves represent data from calculations for $T_0 = 2170$ K, $p_0 = 2.8 \cdot 10^6$ Pa, $p_\infty = 5 \cdot 10^3$ Pa. Since the vibrational temperatures of all the CO_2 modes in the experiments and in the calculations were similar, they represented by single averaged graphs $T_v = f(t)$. While the experimental and calculated results are similar overall, we see that the maximum density of the experimental vibrational temperatures is more elongated and the maximum is more compressed and intense than those of the calculated temperatures.

Figures 2 and 3 shows the time behavior of the vibrational and translational temperatures T_i and T on the axis of the jet at a distance $x = 28\ h_*$ from the nozzle exit, respectively, in mixtures of 9% CO_2 + 91% N_2 and 8% CO_2 + 86% N_2 + 6% H_2O ($T_0 = 2250$ K, $p_0 = 2.8 \cdot 10^6$ Pa). We see that the agreement between the experimental and calculated results is even better for the mixtures than for pure CO_2. The almost complete agreement of the absolute values of the vibrational temperatures as well as their time distribution was unexpected.

The fair agreement between the experimental results and the calculations indicates that the physical model adopted for the processes studied is correct. The computational programs developed can be used to describe a wide range of phenomena associated with unsteady flows of molecular gases.

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