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NUMERICAL MODELING OF PROCESSES IN A RELAXING GAS DURING THE RAPID APPLICATION OF ENERGY

Yu. E. Gorbachev, A. I. Zhmakin,
and A. A. Fursenko

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An important problem of gasdynamics is the investigation of nonsteady processes during the pulsed application of energy to a confined volume of gas. This problem arises, for example, in a study of various types of pulsed-periodic lasers (carbon-dioxide and carbon-monoxide electric-discharge lasers [1-4], exciplex [5], and chemical lasers [6]). The nonuniform character of gasdynamic disturbances is a consequence of the spatial nonuniformity of energy application, which is determined by two circumstances. First, the working volume of a laser usually occupies only part of the channel cross section [3, 7-9]. Second, in gas-discharge lasers the pumping nonuniformity is connected with the complicated character of the distributions of the parameters of the working gas and the electric field, as well as with processes near the electrodes [3, 4]. The nonuniformity of energy application can grow due to the mutual influence of gas heating and gasdynamic processes [1, 3], although this effect is important only in cases when the duration of a pumping pulse is not small compared with the characteristic gasdynamic time.

The determination of shock-wave loads on the channel walls and of the time variation of the uniformity of the working medium is of practical interest. The presence of density disturbances increases the divergence of the radiation [10], and this effect is the more pronounced, the shorter the wavelength. On the other hand, a local density decrease leads to the necessity of reducing the electric field strength, and hence the applied energy, to prevent arcing [4].

A number of papers have been devoted to the theoretical investigation of gasdynamic processes in a channel during rapid energy application, but one-dimensional problems have been considered in the majority of them [1, 11, 12]. In [8] a two-dimensional analysis was made in an acoustic approximation. At the same time, the gasdynamic disturbance cannot be considered as small in the early stages of the process, since the gas pressure can grow severalfold as a result of pumping [4, 5]. The two-dimensional Euler equations are integrated in [3], but since the authors were interested in the influence of gasdynamics on the stability of the discharge, the calculation ends with the end of the pumping pulse (the shock waves have not yet reached the channel walls by this time). In all these investigations a gas with a constant ratio of heat capacities was considered as the working medium. Such a simplification is not always justified: In a carbon-monoxide electric-discharge laser, e.g., the energy stored in vibrational degrees of freedom can exceed the energy of the translational degrees of freedom. In this case, obviously, one must calculate the gas flow with allowance for vibrational relaxation.

We note that the characteristic Reynolds numbers are large in the problem under consideration, and hence the influence of dissipation on the gas dynamics of the flow can be neglected (at least in the initial stage of the process.

1. The purpose of this work is to investigate the influence of various physical effects on the gasdynamic processes in a channel during the rapid application of energy. Usually the

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characteristic size of the working volume in the direction of the optical axis of the resonator is considerably greater than its dimensions in the other directions, so we confine ourselves to the two-dimensional approximation. We consider a plane channel $\Omega = \{0 \le x \le L,\ 0 \le y \le H\}$, a part $\Omega_1 = \{L_1 \le x \le L_2,\ H_1 \le y \le H_2\}$ of which is occupied by the region of energy application. Gas is supplied at an average velocity V_0 through the boundary $x = 0$ and leaves through $x = L$. The walls $y = 0$ and $y = H$ are impermeable. There are several characteristic times in the problem under consideration: the pumping time τ_1, the emission time τ_2 (including the delay time), the characteristic times of acoustic ($\tau_4 = L/a$) and convective ($\tau_3 = L/V_0$) processes (L is the characteristic size and a is the speed of sound), and the interval τ_5 between pulses. As a rule, τ_2 is comparable with τ_1 and $\tau_2 \ll \tau_4$ [2, 4, 7]. Therefore, if we are interested in gasdynamic processes between pulses (rather than the influence of density disturbances on the divergence of the radiation and the stability of the discharge) we can take the energy application as instantaneous.

In a number of installations the working gas is pumped through at a velocity $v_0 \ll a$ [7], so that $\tau_4 \ll \tau_3$, and in an analysis of time intervals on the order of several τ_4 the undisturbed gas can be taken as stationary. We note that in pumping with a Mach number $M_0 = V_0/a$ 1 the shock waves and rarefaction waves interact with the left boundary $x = 0$ of the channel (which actually may be, e.g., a plate with small openings) as with a solid wall.

A special feature of electric-discharge lasers based on molecular gases is the large stock of energy ε_V of vibrational degrees of freedom, which can exceed both the equilibrium vibrational energy ε_V^e and the energy ε_{TR} of translational–rotational degrees of freedom. Therefore, a correct description of the processes requires a joint solution of the equations of gas dynamics and the equations of the populations of vibrational levels. In the case of practical interest, when $_V \gg \varepsilon_V^e$, one must allow for a large number of levels (several dozen). In an exact formulation such a problem is obviously very laborious; in addition, a joint calculation of the vibrational kinetics and the electron distribution function of the volumetric discharge is required to obtain the initial populations [13]. Such a detailed description, required in an investigation of kinetic effects (e.g., the population inversion), is unnecessary in a study of the evolution of gasdynamic disturbances. In the latter case the influence of vibrational relaxation is determined only by the stock of vibrational energy ε_V and the rate W of energy exchange between the vibrational degrees of freedom and the translational and rotational degrees of freedom, in equilibrium with each other. If the form of the distribution function of molecules over the vibrational levels is known, then one can obtain an explicit expression for W dependent parametrically on the gas temperature and the vibrational energy.

Thus, only one equation, describing the variation of vibrational energy, must be added to the equations of continuity, motion, and total energy to close the problem. Let us consider the case of an inviscid, thermally nonconducting gas. The equations in integral form, admitting of continuous solutions, are

$$\frac{\partial}{\partial t}\int_v \rho\, dv + \oint_S \rho \mathbf{V}\cdot\mathbf{n}\, dS = 0; \tag{1.1}$$

$$\frac{\partial}{\partial t}\int_v \rho \mathbf{V}\, dv + \oint_S (\rho \mathbf{V}\mathbf{V} + pI)\mathbf{n}\, dS = 0; \tag{1.2}$$

$$\frac{\partial}{\partial t}\int_v \rho\varepsilon\, dv + \oint_S [(\rho\varepsilon + p)\mathbf{V}]\cdot\mathbf{n}\, dS = 0; \tag{1.3}$$

$$\frac{\partial}{\partial t}\int_v \rho\varepsilon_V\, dv + \oint_S \rho\varepsilon_V \mathbf{V}\cdot\mathbf{n}\, dS = \int_v \rho W\, dv, \tag{1.4}$$

where ρ, $\mathbf{V}$, p, $\varepsilon = \varepsilon_{TR} + \varepsilon_V + (1/2)VV$, ε_{TR}, and ε_V are the density, velocity, pressure, and total, translational–rotational, and vibrational energies; $\mathbf{n}$ is the outward normal to the surface S surrounding the volume v; I is the unit tensor.

The initial conditions are set up as follows: $\rho = \rho_0$ and $\mathbf{V} = 0$ in the region $\Omega \cap \Omega_1$, $\varepsilon_{TR} = \varepsilon_{TR}(T_0)$ and $\varepsilon_V = \varepsilon_V^e(T_0)$ in the region Ω, and $\varepsilon_{TR} = \varepsilon_{TR}(T_*)$ and $\varepsilon_V = \varepsilon_{V_1}$ in the region Ω_1, with $\varepsilon_{V_1} \gtrsim \varepsilon_{TR}(T_*)$ and $\varepsilon_{V_1} \gg \varepsilon_V^e(T_*)$. Here T is the translational–rotational temperature; ε_V^e is the equilibrium vibrational energy.

The condition of nonpenetration is set up at the boundaries $x = 0$, $y = 0$, and $y = H$ and "soft conditions," signifying that the second derivatives of the conservative gasdynamic quantities equal zero, are set up at $x = L$.

We note that some of the simplifications used are not fundamental. Thus, the allowance for the finite pumping velocity with $M_0 \ll 1$ and the finiteness of the time of energy application is trivial, although the latter requires the explicit assignment of the variation of ε_{TR} and ε_V due to pumping and emission.

2. The excitation of a large number of vibrational levels leads to a number of peculiarities in the occurrence of the relaxation process connected with the anharmonicity of the vibrational spectrum of the molecules.

For the diatomic gases of practical interest, efficient VV exchange assures the establishment of a quasisteady distribution over the internal degrees of freedom in a time considerably less than than the characteristic gasdynamic time τ_4. This allows us to use a shortened description for the phenomena under investigation, i.e., to introduce only one additional parameter, the vibrational energy ε_V. The quantity ε_V is defined by the relation

$$\varepsilon_V = N^{-1} \sum_n E_{Vn} f_n, \tag{2.1}$$

where $E_{Vn} = \hbar\omega_e[n + 1/2 - \chi_e(n + 1/2)^2]$ is the energy of the anharmonic oscillator modeling a gas molecule; f_n is the distribution function over the vibrational levels, normalized to the number density N ($\rho = mN$ and m is the mass of a molecule); ω_e is the frequency of the oscillator; χ_e is the anharmonism constant.

The anharmonicity of the molecules results in the fact that at sufficiently low temperatures the quasisteady distribution function established over the levels differs significantly from a Maxwell–Boltzmann distribution and decreases more slowly with level number than the latter. This means an increase in the stock of vibrational energy at the upper levels. Such a distribution was found in analytic form in [14].

Equation (1.4) for $\rho\varepsilon_V$ is obtained by summing the equations for the level populations multiplied by mE_{Vn}. On the right sides, describing the collisional exchange of energy, we neglect the corrections for anharmonicity in the cofactors of E_{Vn} (retaining such corrections in the transition probabilities and in the distribution function). In this case we obtain a "right side" corresponding exactly to the equation for $\hbar\omega_e\rho\alpha$, where $\alpha = N^{-1}\sum_n nf_n$ is the average stock of vibrational quanta per molecule. A determination of ε_V and $\hbar\omega_e\alpha$ on the basis of a solution of the equations of level-by-level kinetics [15] showed that their values differ by 2-3% in the process of relaxation. This allows us to assume that the equation obtained will correctly describe the evolution of the quantity $\rho\varepsilon_V$. As a result, for W in Eq. (1.4) we can use an expression from [14], which we shall not present here because it is cumbersome.

The rate constants of transitions from the initial state i to the final state f used in [14] to calculate W can be represented in the form

$$K_{i\to f} = K_0 F(T, i \to f), \tag{2.2}$$

where K_0 are the constants of the primary transition; F is a scaling factor allowing one to determine all the other constants from K_0. An investigation of such representations [16] showed that the expressions presently in use for K_0 poorly describe the temperature dependence. This is connected with the fact that simplified models, based, as a rule, on collinear collisional dynamics and simple (usually repulsive) interaction potentials, are used to calculate the constants of the primary transitions. But such assumptions about the collisional model prove to be unjustified, since the attractive part of the potential determines the resonance VV processes in practically the entire temperature range of interest. Allowance for the noncollinearity of collisions also alters the temperature dependence of the constants. Moreover, the difference in the translational energy before and after the collision, usually not taken into account, becomes important in the energy decrease of the colliding molecules, resulting in an entirely different form of the constants at temperature less than a certain critical value. On the other hand, the region of applicability of the equations for the scaling factors, calculated within the framework of the standard simplified models, proves to be considerably wider than for the constants of the primary transitions [16]. Therefore, it is natural to use the traditional representations in the calculations of these factors.

In obtaining the expression for the quasi-steady distribution, permitting the calculation of all the other characteristics, we used only the form of the scaling factor, while the constants of the primary transition appear in the final expression in the form of parameters. The difference in the regions of applicabilility of the expressions for K_0 and F allows us to use the representation of [14] for W with refinement only of the parameters P_{10} and Q_{10} of the primary transition in it.

To determine the rate constants we use the results of [17, 18], where a systematic procedure is laid out for calculating the constants for slow (adiabatic) collisions. A variant of the three-dimensional quasiclassical method of calculating the amplitudes of inelastic transitions lies at its foundation. The representations obtained for the constants take into account the noncollinearity of the collisions, the action of the attractive part of the intermolecular potential, and the anharmonicity of the intramolecular vibrations.

These investigations allowed us to reveal the existence of a multitude of different regimes of temperature dependence of the constants (the majority of which had not been isolated before).

First of all, let us consider the constants of VT processes. For the deactivation constant of the first level we can obtain the composite equation [18]

$$P_{10} = 2\sqrt{\frac{\pi}{6}}\,A_0\left(\pi d\omega_e(1-\chi_e)\sqrt{\frac{\mu}{kT}}\right)^{1/3}\left(1-\frac{1}{g}\left(\frac{T_\Delta}{T}\right)^{2/3}\right)^{g}\times$$
$$\times\exp\left[-\frac{3}{2}\left(\frac{\pi^2\mu d^2\omega_e^2(1-\chi_e)^2}{kT}\right)^{1/3}-\frac{\Delta E}{kT}\right]\quad\text{for}\quad T>T_\Delta; \tag{2.3}$$

$$P_{10} = 8\sqrt{\frac{2\pi\mu}{kT}}\,\frac{A_0(\Delta E)^2}{a_0(-2\Delta E-kT)}\left(\frac{4a_0\mu kT}{(-2\mu\Delta E)^{3/2}}\,\frac{\Delta E+2kT}{2\Delta E+kT}-\frac{2\Delta E}{kT}\right)^{-1/2}\times \tag{2.4}$$
$$\times\exp\left(-\frac{-\frac{2\Delta E}{kT}+\frac{a_0\sqrt{-2\mu\Delta E}}{\mu kT}-\frac{a_0}{\sqrt{-2\mu\Delta E}}}{-\frac{2\Delta E}{kT}-1}\right)\quad\text{for}\quad T<T_\Delta,$$

where the characteristic temperature is defined by the relation

$$kT_\Delta=\frac{(2(1-2\chi_e))^{3/2}\hbar}{\pi d(1-\chi_e)}\sqrt{\frac{\hbar\omega_e}{\mu}}, \tag{2.5}$$

$\Delta E = E_j - E_i$, in our case $\Delta E = -\hbar\omega_e(1 - 2\chi_e)$ (for deactivation processes $\Delta E < 0$),

$$g=1+2\,\frac{\sqrt{3(-2\mu\Delta E)^{3/2}}}{a_0^{3/2}e},\quad a_0=\pi\mu d\omega_e(1-\chi_e),$$
$$A_0=\left[\frac{a^{VT}\pi d}{4\hbar}\left(\frac{\mu d\omega_e}{2}(1-\chi_e)-\frac{\sqrt{2\mu D}}{2}\right)\right]^2(2-\chi_e),$$

d and D are parameters of the Morse potential describing the elastic intermolecular interaction; a^{VT} is a binding constant describing the asphericity of the molecule.

In general the VV exchange constants have a very complicated structure [18]. However, at temperatures $T > T_r$, where

$$kT_r=\frac{4}{3}\mu(\omega_e\chi_e d)^2, \tag{2.6}$$

the constant of interest to us is determined by the resonance interaction of the colliding molecules. The temperature T_r for the majority of diatomic gases is low [$T_r(N_2)$ = 170°K, $T_r(CO)$ = 100°K], permitting the use of a single expression for Q_{10}

$$Q_{10}=3\left(\frac{\pi a^{VV}d}{16\hbar}\right)^2(2-\chi_e)(2-3\chi_e)\left[D+\frac{kT}{\pi^2}-\sqrt{\frac{kTD}{\pi}}\right], \tag{2.7}$$

where a^{VV} is the binding constant (the asphericity parameter of the molecules), in the entire temperature range.

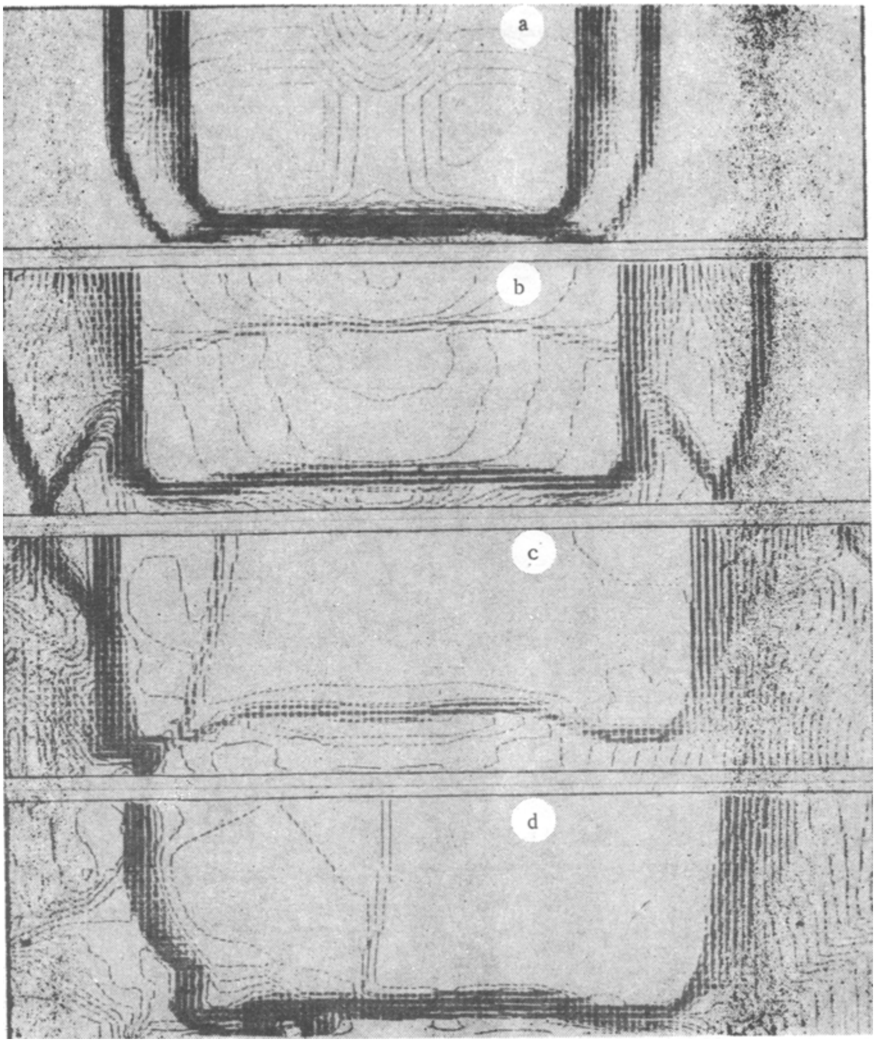

Fig. 1

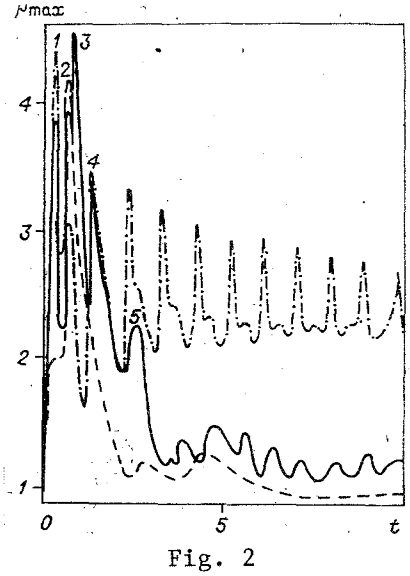

Fig. 2

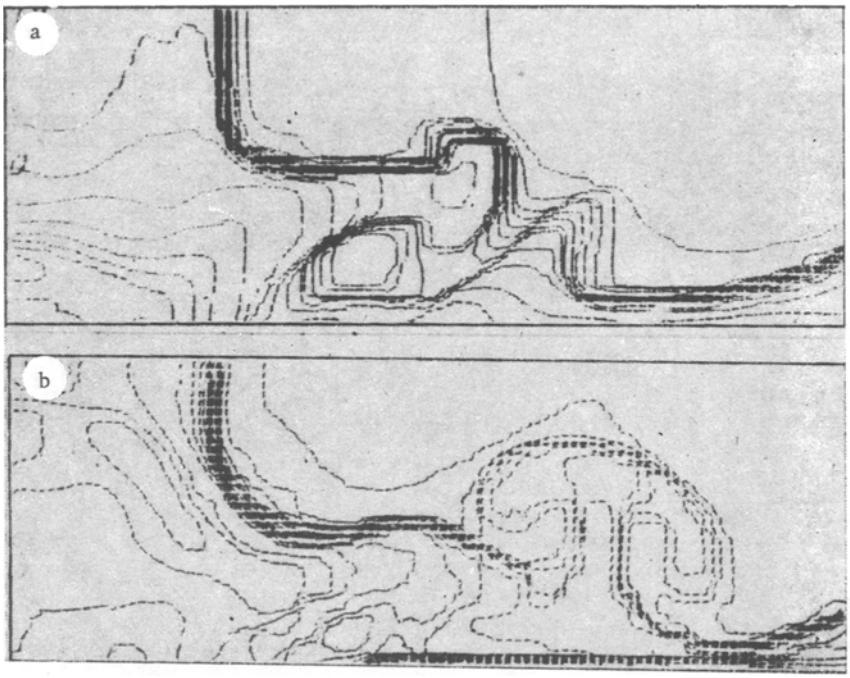

Fig. 3

The results of calculations by Eqs. (2.3) and (2.7) agree well with the data of trajectory calculations in the case of relatively high particle energies (T ≥ 300°K) and with the available experimental data [18].

We also present an expression for the frequency of elastic collisions between particles [their interaction is described by the Lennard-Jones potential (2.2)-(2.8)], using the results of [19] and refining the numerical coefficients:

$$\tau^{-1} = 4N\sigma^2\left[\pi^{0,9}0{,}931\left(\frac{2kT}{\mu}\right)^{0,3}\left(\frac{5D\sigma}{4\hbar}\right)^{0,4} + 2\sqrt{\frac{2\pi kT}{\mu}}\left(0.976 - \frac{1}{6}\ln\left(1 + 0.119\frac{kT}{D}\right)\right)\right], \tag{2.8}$$

where D and σ are parameters of the potential (D is the depth of the potential well).

For the calculations made with CO we took the following values of the parameters appearing in (2.3)-(2.8):

$$\omega_e = 2143\ \text{cm}^{-1},\ \chi_e = 6.23\cdot10^{-3},\ d = 0.485\cdot10^{-10}\ \text{m},\ D = 110^\circ\text{K},$$
$$a^{VT} = 8.13\cdot10^{-2},\ a^{VV} = 0{,}015,\ \sigma = 3.59\cdot10^{-10}\ \text{m}.$$

3. The system described was integrated on a monotonic difference scheme of second-order accuracy, described in detail in [20]. Let us dwell briefly on the realization of the kinetic model. In view of the large number of elementary functions in the expressions for the vibrational energy and the rate of energy exchange, the calculation was begun with the construction of tables of $\varepsilon_V(T_i, T_{1j})$ and $W(T_i, T_{1j})$, $1 \le i \le I$, $1 \le j \le J$ (as a rule, we took I = 30-40 and J = 100).

The values of $\varepsilon(T, T_1)$ and $W(T, T_1)$ required in the process of solution were found by linear interpolation. The expenditures of computer time grew by 1.6 times compared with a calculation of the flow of an ideal gas.

Let us examine the development of the flow on the example of an ideal gas ($T_*/T_0 = 5$, $\Omega_1 = \{1 \le x/L \le 2.2,\ 0.3 \le y/L \le 1\}$). In Fig. 1a-d we present lines of constant density with a step $\delta\rho/\rho_0 = 0.05$ at the times t = 0.28, 0.56, 1.12, and 1.4, respectively.

A shock wave, a contact discontinuity, and a rarefaction wave are formed in the decay of a two-dimensional gasdynamic discontinuity. At the time t = 0.28 the shock wave was reflected from the lower wall and by the time t = 0.56 the reflection changes to the irregular type. The shock wave moving toward the right leaves the channel at t ≈ 1, while the other "longitudinal" shock wave, after reflection from the left wall, interacts in a complex way with the contact discontinuity and the rarefaction wave (Fig. 1c and d).

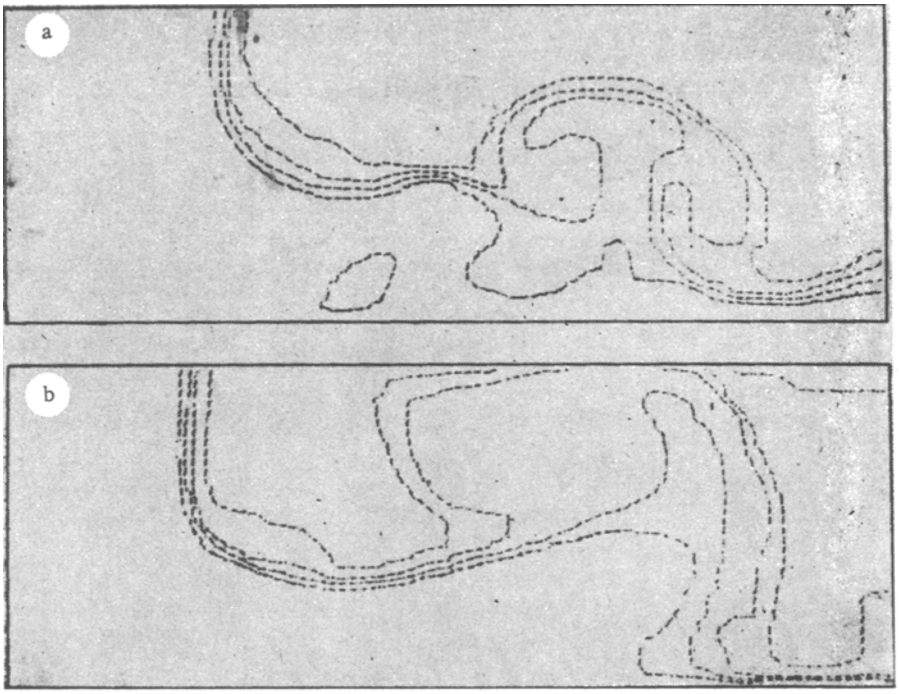

Fig. 4

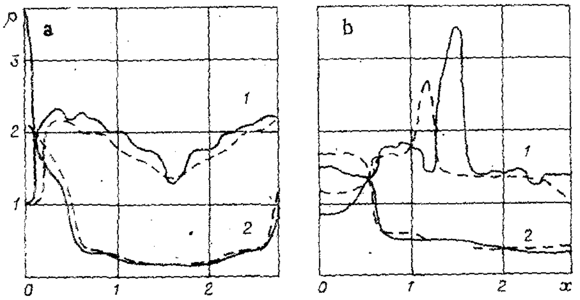

Fig. 5

The comparison of the two-dimensional (solid curve) and one-dimensional calculations (dashed curve) presented in Fig. 2 shows the decisive role of transverse shock waves in the damping of gasdynamic disturbances; here we also present the time dependence of the maximum gas density in the working volume. The first maxima on the curve obtained in the two-dimensional calculation are easy to identify. They correspond to the reflection of the shock wave from the lower wall (1), the reflection from the left wall of the upper part of the shock wave (2) and of the Mach foot (3), the reflection from the upper wall (4), and the interaction of the shock wave with the contact discontinuity (the right boundary of the hot region) (5). It is seen that the second and fifth maxima also occur in the one-dimensional calculation. The time variation of the maximum density for purely transverse shock waves ($\Omega_1 \equiv \{0 \leq x/L \leq \infty,\ 0.3 \leq y/L \leq 1\}$), represented by a dash-dot line in Fig. 2, shows that the influence of approximation errors on the damping of gasdynamic disturbances is insignificant.

Because of the interaction with reflected shock waves the region of hot gas takes a rather complicated shape. In Fig. 3 we show isopeaks at the time $t = 5.6$ for frozen-in (a) and nonequilibrium (b) flows ($T_0 = 120°K$, $\alpha_0 = 0.25$). Lines of ε_V = const for the latter case are shown in Fig. 4a and b at the times $t = 5.6$ and 12.3, respectively.

In Fig. 5 we present a comparison of the density distributions along the lower (curves 1) and upper (curves 2) walls for the cases of nonequilibrium (solid lines) and frozen-in (dashed lines) flows at the times $t = 0.56$ (a) and 1.4 (b). It is seen that relaxation processes have a lesser influence on the flow structure (at least at the initial times) and a greater influence on the intensity of gas motions. This conclusion is supported by Fig. 6,

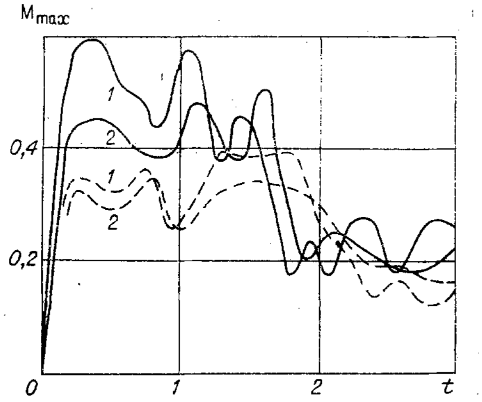

Fig. 6

where the time variation of the maximum Mach number is shown. The solid curves correspond to $\alpha_0 = 1$ and the dashed curves to $\alpha_0 = 0.5$; $T_*/T_0 = 2$ and $T_0 = 150°K$. Curves 2 differ from curves 1 by a fivefold decrease in pressure. It is seen that a decrease in the relaxation rate leads to the fact that the maximum velocities are observed not at the initial times of decay of the gasdynamic discontinuity, as in the case of an ideal gas, but considerably later. The sharp decrease in M at times on the order of 1.5-2 corresponds to the emergence from the channel of the shock wave reflected from the left wall. As one would expect, this occurs the earlier, the larger α_0 and the higher the pressure.

In conclusion, we note that the difference grids used in the calculations contained about 3000 cells. The calculation time per cell in one time step was 9 msec on a BESM-6 computer.

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PROPAGATION OF A RADIATION PULSE WITH WAVELENGTH $\lambda = 10.6$ μm IN AMPLIFYING MEDIA

V. A. Levin, V. V. Netesov,
and A. M. Starik

UDC 535+534.222+539.196

Investigations of radiation amplification processes in multistage CO_2 amplifiers have recently intensified. Information about both the amplitude and phase characteristics of the radiation being amplified is necessary here to obtain high-intensity laser radiation in the far zone and small beam divergence.

Heating of the gas occurs in propagation of a collimated beam through a CO_2–N_2 amplifying medium because of the induced transitions from the level 00°1 to the level 10°0 and the subsequent vibrational–translational relaxation of the vibration energy of the CO_2 molecules. Moreover, because of the inhomogeneity in the intensity distribution over the beam radius (there is usually a Gauss distribution), thermalization of the gas over the beam radius will also occur nonuniformly.

Subsequently, the inhomogeneous temperature field will result in a nonuniform change in the refractive index over the beam radius, and will defocus the beam being propagated through the amplifying medium.

The influence of these processes on the amplitude–phase characteristics of the radiation being amplified was first investigated in [1]. However, questions of the influence of the possible inhomogeneity of the medium (particularly the inhomogeneity in the gain over the beam radius), and also of certain features of the vibrational-energy transfer processes on the radiation characteristics were not considered here.

On the basis of numerical modeling, propagation of a pulse of electromagnetic radiation with $\lambda = 10.6$ μm through a CO_2–N_2–He amplifying medium with both a uniform and a nonuniform parameter field in the beam channel is examined here. Singularities in the production of the active medium are not taken into account here, and influence of the motion of the medium was assumed inessential.

The analysis was performed for pulses whose duration τ_I is much greater than the rotational–translational (τ_{R-T}), vibrational–vibrational (τ_{V-V}) relaxation times, and greater than the characteristic hydrodynamic time of the problem τ_p (the time of acoustic vibrations propagation across the beam) but less than the free convection, molecular diffusion, and heat conduction times. In this case, assumptions about the presence of a local Boltzmann distribution in each separate type of CO_2 and N_2 molecular vibration and on the existence of thermodynamic equilibrium between the translational and rotational motion of the mixture molecules are valid [2].

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