OPTIMIZATION OF THE PARAMETERS OF A CO_2 GASDYNAMIC LASER

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In order to maximize the gain coefficient of a CO_2-N_2-He gasdynamic laser, a total optimization of the stagnation parameters, the concentration coefficient, and the parameters which determine the shape of the nozzle (assuming a quasi-one-dimensional flow model) was carried out. The dependence of the optimized parameters on the limitations imposed by the stagnation temperature of the flow and the critical cross section have been determined.

Solutions for the population inversion of CO_2 molecules and the gain coefficient for a gas mixture consisting of CO_2, N_2, He, and H_2O expanded by a nozzle have been discussed by many authors [1-11] (see also the references in these works).

The basic assumptions have been established for the determination of the rotational–rotational and rotational–translational exchange processes in these mixtures.

The composition and stagnation parameters of the gas mixture, however, have been varied for fixed nozzles. The results of theoretical solutions, obtained previously, agree well with the experiments. The results of these computations and a series of experiments have been successful in pointing out which quantities depend on the inverted population and the gain coefficient, and the degree of their effect. To a much lesser degree, the range of values of the stagnation parameters, the concentration component of the gas mixture, and the nozzle parameters, which are all necessary in order to obtain the results at conditions near optimal, have been determined.

In order to determine the gain coefficient to a much higher accuracy, it is necessary to include the optimization of the stagnation parameters of the gas mixture and the contour of the nozzle which is used.

In this paper, rotational relaxation is examined in the CO_2-N_2-He mixture, for which the following reaction scheme has been assumed.

The rotational–rotational exchange for the collision of CO_2 molecules with some molecule between the ν_1-, ν_2-, and ν_3- modes progresses as follows:

$$h\nu_3 \rightleftarrows h\nu_1 + h\nu_2 + \Delta E_1 \tag{1}$$
$$h\nu_3 \rightleftarrows 3h\nu_2 + \Delta E_2 \tag{2}$$
$$h\nu_1 \rightleftarrows 2h\nu_2 + \Delta E_3 \tag{3}$$

For the collision of CO_2 molecules with N_2 molecules, the exchange of rotational energy proceeds according to

$$h\nu_3 \rightleftarrows h\,\nu_4 + \Delta E_4 \tag{4}$$

The exchange of energy between the rotational and translational–rotational motion for the CO_2 and N_2 molecules struck by some molecules proceeds as

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$$h\nu_2 \rightleftarrows \Delta E_5 \tag{5}$$

$$h\nu_4 \rightleftarrows \Delta E_6 \tag{6}$$

Here ν_1, ν_2, ν_3, and ν_4 are the characteristic frequencies of the symmetrical valence bond of the doubly-degenerate deformation and the asymmetrical valence bond type of the rotational molecules of CO_2 and N_2, respectively; ΔE_i is the value of the energy of the translational–rotational motion for the corresponding processes.

We will make use of the usually accepted and substantiated assumptions in other papers. First we will assume that inside each partially rotational degree of freedom of the CO_2 and N_2 molecules, there exists a local thermodynamic equilibrium (each mode is interpreted as an oscillator with an infinite number of steady-state levels). For this case, each rotational mode can have a corresponding rotational temperature $T_i (i = 1, \ldots, 4)$. Second, we will assume that $T_1 = T_2$ and $\theta_1 = 2\theta_2$ $(\theta_i = h\nu_i/k)$. This is caused by the strong resonant interaction (3) due to the closeness of the energy of the first level of the ν_1- mode and the second level of the ν_2- mode (Fermi resonance). Third, we will assume that the gas is ideal, neglecting such effects as viscosity, thermal conductivity, and diffusion.

As is usually done, we will also assume that the rotational degrees of freedom are excited classically.

The equations for the conservation of mass and impulse energy and the equation for the state of the quasi-one-dimensional flow model assume the form

$$A\rho u = A_* \rho_* u_* \tag{7}$$

$$\rho u \frac{du}{dx} + \frac{dP}{dx} = 0 \tag{8}$$

$$\left(\frac{5}{2} + \alpha_1 + \alpha_2\right) kT + \alpha_1 \sum_1^3 h\nu_i \varepsilon_i + \alpha_2 h\nu_4 \varepsilon_4 + \frac{mu^2}{2} = \text{const} \tag{9}$$

$$p = \rho \frac{k}{m} T \tag{10}$$

This is a closed system for the relaxation equations, which, allowing for the above-mentioned assumptions, has the form

$$\frac{d\varepsilon_2}{dx} = \frac{2\rho}{mu}(1+\varepsilon_2)^2 (3\varepsilon_2^2 + 6\varepsilon_2 + 2)^{-1} \left[\sum_1^3 \alpha_j K_j (2 \to 0)(1 - e^{-\theta_2/T})(\varepsilon_{02} - \varepsilon_2) - \frac{3}{8}(\varphi_1 + \varphi_2)\right] \tag{11}$$

$$\frac{d\varepsilon_3}{dx} = \frac{\rho}{mu}\left[\frac{1}{8}(\varphi_1 + \varphi_2) + \alpha_2 \varphi_3\right] \tag{12}$$

$$\frac{d\varepsilon_4}{dx} = \frac{\rho}{mu}\left[\sum_1^3 \alpha_j K_j (4 \to 0)(1 - e^{-\theta_4/T})(\varepsilon_{04} - \varepsilon_4) - \alpha_1 \varphi_3\right] \tag{13}$$

$$\varphi_1 = \sum_1^3 \alpha_j K_j (3 \to 2)[\varepsilon_2^3 (1+\varepsilon_3) e^{-\Delta E_2/kT} - \varepsilon_3 (2+\varepsilon_2)^3]$$

$$\varphi_2 = (1+\varepsilon_2)^{-1} \sum_1^3 \alpha_j K_j (3 \to 1, 2)[\varepsilon_2^3 (1+\varepsilon_3) e^{-\Delta E_1/kT} - \varepsilon_3 (2+\varepsilon_2)^3]$$

$$\varphi_3 = K(3 \to 4)[\varepsilon_4 (1+\varepsilon_3) e^{-\Delta E_4/kT} - \varepsilon_3 (1+\varepsilon_4)]$$

Here α_j $(j = 1, 2, 3)$ is the molar concentration of CO_2, N_2, and He, respectively; ρ, u, T, P, and A are the density, velocity, temperature, gas pressure, and cross-sectional area of the nozzle, $m = \sum_1^3 m_j \alpha_j$; m_j is the mass of the j-th type of molecule; $\varepsilon_2 = 2(e^{\theta_2/T_2} - 1)^{-1}$; $\varepsilon_3 = (e^{\theta_3/T_3} - 1)^{-1}$; $\varepsilon_4 = (e^{\theta_4/T_4} - 1)^{-1}$; the quantity ε_{0i} corresponds to the value of ε_i for $T_i = T$; $K_j(3 \to 1, 2)$, $K_j(3 \to 4)$, $K_j(2 \to 0)$, and $K_j(4 \to 0)$ are the rates of the respective reactions (1), (2), (4)-(6) for unit molecular concentrations. The values of the reaction rates have been approximated according to [13, 14].

The surface of the diffuser part of the axisymmetrical nozzle is given in the form

$$A(x) = \begin{cases} A_* + ax^2 + bx^3, & 0 \leqslant x \leqslant l \\ A(l) + 2(x-l)\sqrt{cA(l)} + c(x-l)^2, & x > l \end{cases} \tag{14}$$

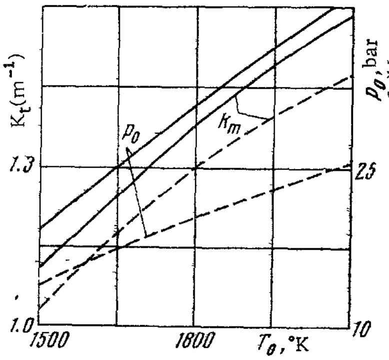

Fig. 1

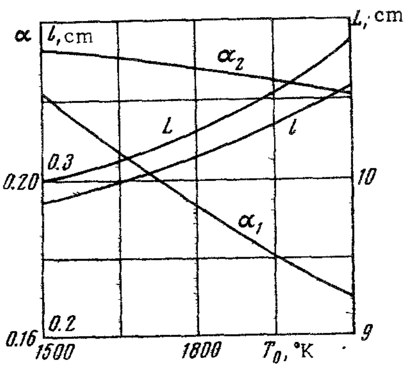

Fig. 2

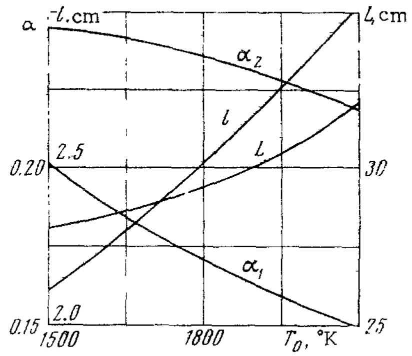

Fig. 3

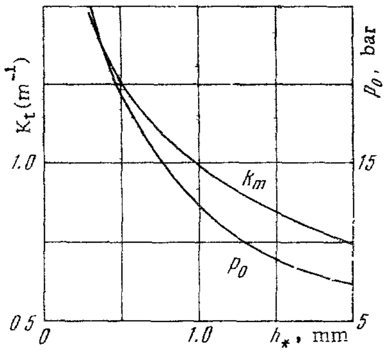

Fig. 4

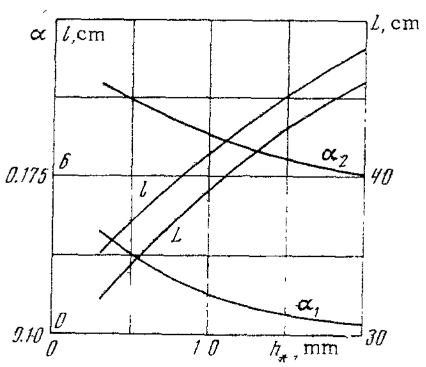

Fig. 5

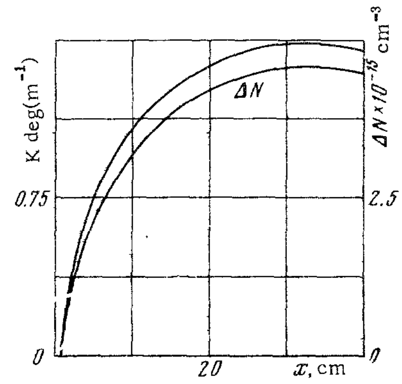

Fig. 6

where x is the distance from the critical cross section downstream along the flow direction; l is the coordinate of the point where the nozzle becomes conical with an angle to the axis of the nozzle of θ; $c = \pi \tan^2\theta$.

Except for [1, 7, 8], where hyperbolic nozzles were studied, a term of the order of x^3 is introduced, whose coefficient is determined from the coupling conditions of the rapid expansion and conical parts of the nozzle. The converging part of the nozzle can be considered as a circle whose radius equals the diameter of the critical cross section.

For a plane symmetrical nozzle, one must choose

$$h(x) = \begin{cases} h_* \sqrt{1 + a(x/h_*)^2 + b(x/h_*)^3}, & 0 \leqslant x \leqslant l \\ h(l) + c(x - l), & x > l \end{cases} \tag{15}$$

where h_* is the height of the slot, l is the transition point of the rapid expansion part of the nozzle in the tapered region with a half angle at the apex θ, and $c = z \tan\theta$. The coefficient b is chosen depending on the conditions in the rapid expansion region ($0 \leq x \leq l$) and tapered region ($x > l$) of the nozzle.

The small signal gain coefficient (absorption) at the center of the line takes the form

$$k^\circ = \frac{\lambda^2 A_{VJ}^{V'J'}}{8\pi \sqrt{\pi} c} \frac{\delta}{\Delta\nu_c} = \left[n_{V'J'} - \frac{g_{V'J'}}{g_{VJ}} n_{VJ} \right] H(\delta, 0) \tag{16}$$

where $n_{V'J'}$, n_{VJ}, $g_{V'J'}$ and g_{VJ} are the populations and statistical weights of the upper and lower laser levels, respectively; $A_{VJ}^{V'J'}$ is the Einstein coefficient for a spontaneous transition from $V'J' \rightarrow VJ$, λ is the wavelength of the transition, c is the speed of light, $\Delta\nu_c$ is the collisional half-width of the line, $H(\delta, 0)$ is the value of the Voigt profile at the center of the line, and $\delta = \Delta\nu_c (\ln 2)^{1/2}/\Delta\nu_\partial$ where $\Delta\nu_\partial$ is the Doppler half-width of the line determined by

$$\Delta\nu_\partial = \left(\frac{2RT \ln 2}{\mu} \right)^{1/2} \frac{1}{\lambda c} \tag{17}$$

Here R is the universal gas constant, and μ is the molecular weight of CO_2. Measurements [17] have shown that $\Delta\nu_c \sim T^{-1}$ in the region $300 \leq T \leq 420°K$ and not $\Delta\nu_c \sim T^{-1/2}$ as is usually assumed. Then it is possible to write

$$\Delta\nu_c = P \frac{300}{T} \sum \delta^\circ_{CO_2-j} \alpha_j \tag{18}$$

Here $\delta^\circ_{CO_2-j}$ is the collisional half-width of the CO_2 line at $T = 300°K$ and at atmospheric pressure of the j-th gas. The population of the lasing levels is determined by the expression

$$n_{VJ} = 2N_V \left(\frac{hcB_V}{kT} \right) g_J \exp\left[-\frac{hcB_V}{kT} J(J+1) \right] \tag{19}$$

where N_V is the total number of molecules at the lasing level, and B_V is the rotational constant of the quantum level.

We will assume that the fundamental contribution to the gain leads to the P(20) transition ($J' = 19$, $J = 20$) band $00°1$–$10°0$ of the CO_2 molecule. The values $A_{10°0,20}^{00°1,19} = 0.169$ sec^{-1}, $\delta^\circ_{CO_2-CO_2} = 0.0832$ cm^{-1}·atom^{-1}, $\delta^\circ_{CO_2-N_2} = 0.0695$ cm^{-1}·atom^{-1}, $\delta^\circ_{CO_2-He} = 0.0576$ cm^{-1}·atom^{-1}, $B_{10°0} = 0.3897$ cm^{-1}, and $B_{00°1} = 0.3866$ cm^{-1} were taken from [16, 18]. Now the optimization problem leads to a determination of

$$k_m = \max_{a_i \in M} (\sup_x k^\circ(x)) = \max_{a_i \in M} G$$

where M is the region of valid values of the optimization paramaters, a_i are the parameters to be optimized (α_1, α_2, T_0, P_0, a, A_*, l, θ) and G is an optimized functional, $G \equiv \sup_x k^\circ(x)$.

The concentration limit of the components of the lasing mixture is determined by the natural form

$$0 \leqslant \alpha j \leqslant 1, \quad \sum_1^3 \alpha_j = 1$$

The upper limits of the stagnation parameters vary up to a temperature $T = 2100°K$ and $P_0 = 200$ atm. The lower limits of the values A_* and h_* also vary. The upper limit of the parameter a, which determines the shape of the nozzle, is chosen so that the maximum angle with respect to the axis of the nozzle is not larger than 18° for plane nozzles, and 15° for axisymmetric nozzles.

The solution of the problem is carried out by a differential method. Previously, from Eqs. (7)-(10) we obtained

$$\frac{du}{dx} = u\left[\frac{T}{A}\frac{dA}{dx} + \frac{1}{\beta}\left(\alpha_1 \sum_1^3 \theta_i \varepsilon_i + \alpha_2 \theta_4 \varepsilon_4 \right) \right] \left[\frac{\beta - 1}{\beta} \frac{m}{k} u^2 - T \right]^{-1} \tag{20}$$

where $\beta = 5/2 + \alpha_1 + \alpha_2$. The system of equations (7), (9)-(13), and (20) are integrated again. The previous solutions, as in [1, 6, 9], have initially showed that the flow remains in equilibrium for all practical purposes right up to the point given by Eq. (20) for relatively low pressures. Therefore, integration for further solutions can begin right at this point. Second, Eqs. (11)-(13) determine the maximum slit height which will also guarantee the specified accuracy of the computation, and this value, although very small in the near-equilibrium region, increases significantly in proportion to the deviation from equilibrium. This has a limiting effect on the selection of a maximum possible interval in the first integral and its increase in further integration. All this leads to the possibility of reducing the computer time by one iteration for integrating by the Runge–Kutta method on the BÉSM-6 computer to 20-30 sec. A sufficiently accurate determination of the optimization requires 20-30 iterations.

In Fig. 1 the dependence of the optimum values of the stagnation pressure and the dependence of the maximum gain coefficient on the stagnation temperature are shown. The solid curves are for the axisymmetric nozzle ($A_* = 0.1$ mm^2), and the dashed curve is the plane nozzle ($h_* = 0.3$ mm). In Fig. 2 (axisymmetric nozzle, $A_* = 0.1$ mm^2) and Fig. 3 (plane nozzle, $h_* = 0.3$ mm) are shown the dependences of the stagnation temperature for the optimum values of the component concentrations of the gas mixture α_1 and α_2, the coordinates of the transition points of the nozzle in the cone (wedge) l, and the coordinate L at which the maximum value of $k°$ is reached. The dependences of these same quantities on the critical velocity in the plane nozzle at $T_0 = 2100°K$ are shown in Figs. 4 and 5. Measurements of the gain coefficient and the inverted population ($\Delta N = N_{00°1} - N_{01°0}$) along the length of the nozzle, beginning at the critical cross section for the optimal case, are shown in Fig. 6 for a plane nozzle, $T_0 = 2100°K$ and $h_* = 0.3$ mm.

In all cases the optimum appears to be distributed at the lower limits of values of h_* and θ and at the upper limits of the parameter a and stagnation temperature T_0.

The results of the calculations presented show that, for complete optimization of all the parameters, it is possible to obtain a gain coefficient of about 0.015 cm^{-1} at rather moderate values of the stagnation parameters. A further increase in the gain coefficient in the $CO_2 - N_2 -$He mixture is possible when a broader class of nozzle is considered.

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