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CALCULATION OF CHEMICAL- AND VIBRATIONAL-NONEQUILIBRIUM FLOW OF A MULTICOMPONENT GAS THROUGH A NOZZLE

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INTRODUCTION

The calculation of the flow of a multicomponent gas mixture under certain conditions requires the joint allowance for the kinetics of the chemical reactions and the processes of vibrational energy exchange. Until now, however, such calculations have not been made in a sufficiently general formulation, and this is explained both by the complexity of the mathematical solution and by difficulties connected with the systematic formulation of the problem and the absence of data on many of the kinetic characteristics, particularly those describing the interaction of the processes of chemical and vibrational kinetics.

In practice one usually assumes that the separation of these processes is possible. Under specific conditions this can actually be justified. For example, for nozzles of relatively large diameters and with high reservoir temperatures ($T_0 \sim 3000°K$), such as in application to the calculation of the flow parameters in rocket engine nozzles (see the review in [1], for example), it is sufficient to allow for only the chemical nonequilibrium, assuming in this case that the vibrational degrees of freedom of the molecules are in equilibrium with the translational degrees of freedom. The soundness of such an approach is due both to the

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relative validity under these conditions of the relation

$$\tau_r \sim \tau_f \gg \tau_q, \tag{0.1}$$

and the relative smallness of the supply of vibrational energy in comparison with the chemical energy ($\Delta H_V < 30\% \, \Delta H_C$) (here τ_f, τ_r, and τ_q are the characteristic times for the flow, the chemical reactions, and the vibrational relaxation).

In calculations of nonequilibrium flows in application to gasdynamic CO_2 lasers (nozzles of small diameters, $T_0 \lesssim 2500$°K; see the review [2], for example) it is sufficient to allow for only the vibrational nonequilibrium, taking the chemical composition as constant in accordance with the relation

$$\tau_r \gg \tau_f \sim \tau_q. \tag{0.2}$$

The assumption (0.2) is actually justified for relatively simple systems (a CO_2–N_2–He mixture was being considered). This is indicated by the results of the calculations of [3, 4], in which the kinetics of the nonequilibrium recombination of the CO_2 was taken into account along with the vibrational nonequilibrium.

A tendency toward an increase in the temperatures and pressures in the reservoirs of gasdynamic lasers (GDL) and a complication of the laser mixtures (addition of water and other components, the use of fuel combustion products as the working substance) has been revealed in recent years. Under these conditions the relation (0.2) may no longer be satisfied (mainly due to the presence in complex mixtures of a large number of fast bimolecular exchange reactions), and the processes of chemical and vibrational kinetics must be analyzed jointly.

For kinetic problems formulated both with the use of (0.1) or (0.2) and without their use, the difficulties of a mathematical nature are general and for the most part have been overcome by now [1].

The problem of the calculation of the chemical- and vibrational-nonequilibrium flow of a multicomponent gas mixture through a nozzle is formulated in the present report on the basis of the use of a number of simplifying assumptions. An implicit scheme, first applied to calculations of chemical kinetics in [5], is used for the solution of the problem. The results of numerical calculations for a mixture of the elemental composition H–O–C–N, illustrating the interaction of the chemical and vibrational nonequilibrium, are presented.

1. STATEMENT OF THE PROBLEM

For a whole series of applications it is sufficient to determine the stream parameters (T, ρ, p), the concentrations n_i of the individual components, and the average energies ε_k of the vibrational degrees of freedom. This circumstance considerably simplifies the formulation of the kinetic equations, permitting the use of the following simplifying assumptions: a) The chemical reactions do not disturb the Maxwell distribution; b) the rotational degrees of freedom are in equilibrium with the translational degrees of freedom; c) each type of molecular vibrations (mode) is modeled by a harmonic oscillator; d) $\tau_{VV} \ll \tau_{VT}$, $\tau_{VV'}$, τ_r (τ_{VV}, $\tau_{VV'}$, and τ_{VT} are the characteristic times of energy exchange within one mode, between different modes, and of vibrational–translational exchange, respectively). The latter assumption permits the introduction of the concept of the vibrational temperature T_k as a measure of the average energy of one or another mode (such as the k-th).

A systematic derivation of the kinetic equations for the average vibrational energies ε_k from the equations of population balance of the vibrational levels without allowance for chemical reactions on the assumptions b), c), and d) was carried out in [6]. The variation in the concentrations of the components is described by the usual phenomenological equations of chemical kinetics, with the effect of the process of vibrational relaxation on the kinetics of the chemical transformations being expressed through the dependence of the rate constants of the reactions on the vibrational temperatures of the corresponding modes. But the effect of the chemical reactions on the process of vibrational relaxation entails the appearance of an additional term on the right sides of the equations of vibrational kinetics [7, 8]. The direct application of the results of [6-8] to the case of a multicomponent gas mixture leads to the following equations for the molar concentrations n_i of the components per unit mass and the average numbers ε_k of vibrational quanta of the modes:

$$\frac{dn_i}{dt} = \sum_{r=1}^{L_1} (\nu'_{ir} - \nu_{ir})(R_r - R'_r), \tag{1.1}$$

$$R_r = k_r \prod_{j=1}^{N} (\rho n_j)^{\nu_{jr}},\ R'_r = k'_r \prod_{j=1}^{N} (\rho n_j)^{\nu'_{jr}};$$

$$\frac{d\varepsilon_k}{dt} = \sum_{q=1}^{L_2} l_{kq} \sum_{i=1}^{N} Z_{ji} P_{ji}^{(q)} \prod_m \left(\frac{l_{mq} + \lambda_m \sigma_{ji} - 1}{l_{mq}}\right)(Q_q - Q'_q) +$$

$$+ \sum_{r=1}^{L_1} (\nu'_{jr} - \nu_{jr})\left[(\chi_{rk} - \varepsilon_k) R_r - (\chi'_{rk} - \varepsilon_k) R'_r\right]/\rho n_j, \tag{1.2}$$

$$Q_q = \prod_m \left[\frac{\varepsilon_m^0 (\lambda_m + \varepsilon_m)}{\lambda_m (\lambda_m + \varepsilon_m^0)}\right]^{l_{mq}} \prod_n \left[\frac{\varepsilon_n (\lambda_n + \varepsilon_n^0)}{\lambda_n \varepsilon_n^0}\right]^{l_{nq}},$$

$$Q'_q = \prod_m \left(\frac{\varepsilon_m}{\lambda_m}\right)^{l_{mq}} \prod_n \left(\frac{\lambda_n + \varepsilon_n}{\lambda_n}\right)^{l_{nq}},$$

k = 1, 2, ..., S (the mode k pertains to the molecule j).

Here k_r (k'_r) is the rate constant of the r-th reaction in the forward (reverse) direction; $P_{ji}^{(q)} = P_{ji}\begin{Bmatrix} l_{mq} \to 0 \\ 0 \to l_{nq} \end{Bmatrix}$ is the probability of the q-th vibrational transition during one collision of molecules of the i-th and j-th types; ν_{ir} and ν'_{ir} are the stoichiometric coefficients of the i-th component in the r-th reactions; Z_{ji} is the number of collisions of molecules of type i with molecules of type j per unit time with a unit concentration of the former; $\varepsilon_k^0 = \varepsilon_k(T)$; λ_k is the degree of degeneration of the k-th mode; L_1 and L_2 are the total numbers of chemical reactions and of channels of vibrational relaxation, respectively;

$$\sigma_{ij} = \begin{cases} 2 & \text{for } j = i \\ 1 & \text{for } j \neq i; \end{cases}$$

N is the number of components in the mixture; S is the total number of modes; χ_{rk} (χ'_{rk}) is the average number of vibrational quanta obtained (lost) by the k-th mode in one act of formation (annihilation) of a molecule of type j in the r-th reaction, where the forward direction of the reaction is taken as that in which molecules of type j are formed,

$$\chi_{rk} = (E_r/\hbar\omega_k)\,\eta_{kr},\ \chi'_{rk} = (E_r/\hbar\omega_k)\,\eta'_{kr}; \tag{1.3}$$

$$k_r(T, T_k) = \varkappa_r(T, T_k)\, k_r^0(T), \tag{1.4}$$

where $k_r^0(T)$ is the rate constant of the r-th reaction in thermodynamic equilibrium; ω_k is the frequency of the k-th vibration; E_r is the portion of the activation energy of the r-th reaction belonging to the vibrational degrees of freedom. In accordance with the assumptions a) and b), for the quantity E_r at high enough temperatures (the translational and rotational motion are analyzed classically) one can take

$$E_r = E_r^A - (\xi_r + 3)\,kT/2, \tag{1.5}$$

where E_r^A is the activation energy of the r-th reaction in the direction of annihilation of the molecule containing the k-th mode (the energy of bond breaking in the dissociation reactions); ξ_r is the number of rotational degrees of freedom of the molecules participating in the r-th reaction. Although Eq. (1.5) has a rough estimating character, for the temperatures under consideration it is in qualitative agreement with the available experimental data for bimolecular exchange reactions [9] and in satisfactory quantitative agreement for dissociation reactions [10]. In the case of a dissociation reaction [7, 8]

$$\eta'_{kr} = \beta_{rk}^2 T_k^2 \sum_i \beta_{ri}^2 \Big/ \Big(\sum_i \beta_{ri}^2 T_i\Big)^2,\ \eta_{kr} = \beta_{rk}^2 \Big/ \sum_i \beta_{ri}^2; \tag{1.6}$$

$$\varkappa_r(T, T_k) = \exp\left[\frac{E_r}{k}\left(\frac{1}{T} - \frac{\sum\limits_i \beta_{ri}^2}{\sum\limits_i \beta_{ri}^2 T_i}\right)\right] \tag{1.7*}$$

(β_{ri} are the coefficients of the resolution of the reaction coordinates along the normal coordinates). Due to the lack of information on β_{ri} the latter are assumed to be equal to each other in the majority of cases. As a first approximation for bimolecular exchange reactions one takes $\eta_{1r} = \eta_{2r} = \ldots = 1/b_r$, where b_r is the number of modes participating in the r-th reaction; one can use Eq. (1.7) to estimate $\varkappa_r$ or one can set $\varkappa_r = 1$.

The gasdynamic equations are standard for such calculations — the flow is steady and one-dimensional and viscosity, heat conduction, and diffusion are ignored:

$$\begin{gathered} \rho v A = G; \frac{dp}{dx} = -\rho v \frac{dv}{dx}; \ p = n\rho RT; \\ n = \sum_{i=1}^{N} n_i; H + \frac{1}{2} v^2 = H_0; H = \sum_{i=1}^{N} H_i n_i. \end{gathered} \tag{1.8}$$

Here x is the coordinate along the nozzle axis; A = A(x) is the cross-sectional area of the nozzle; G is the mass flow rate; v is the stream velocity; R is the universal gas constant; $H = H(T_k, T, p)$ is the enthalpy of a unit mass of the gas mixture; H_0 is the stagnation enthalpy; and H_i is the molar enthalpy of the i-th component.

Thus, for the flow of a vibrationally and chemically nonequilibrium multicomponent gas mixture we have a closed system of N + S + 4 equations (1.1), (1.2), and (1.8) relative to the same number of unknowns n_i, ε_k, p, v, ρ, and T.

2. CALCULATION METHOD

In the present report the initial system of equations is divided into two subsystems: kinetic) Eqs. (1.1) and (1.2) with (1.3)-(1.7) (subsystem I) and gasdynamic) Eqs. (1.8) (subsystem II), with the solution of the gasdynamic subsystem being reduced to the integration of the equation for the function $F = A(x)p/G + v$:

$$\frac{dF}{dx} = \frac{1}{G} p \frac{dA}{dx}. \tag{2.1}$$

The temperature T at each step of integration is determined from the equation

$$F/2 \pm \sqrt{F^2/4 - nRT} - \sqrt{2(H_0 - H)} = 0. \tag{2.2}$$

The commencement of the calculation from the subsonic region along with the assignment of a dependence A = A(x) leads to the appearance of a singlular point of the "saddle" type. Therefore, the mass flow rate is chosen by iteration and the subsonic and supersonic branches of the solution which are realized physically are joined at the singular point.

The kinetic subsystem is integrated using an implicit difference scheme of the first order of approximation with subsequent application of Newton's method. Such a scheme was first used in [5] to integrate equations of chemical kinetics. However, the application of this scheme to the entire system of equations (1.1)-(1.8) is difficult when Eq. (2.1) is used because of the ambiguity of the solution of Eq. (2.2) in the region of the singular point, and therefore Eq. (2.1) is integrated by Euler's method with recalculation. Instead of a numerical solution of (2.2) at each step in x the enthalpy of the mixture is represented in the form $H = C_0T + C(T_k)$. This permits a conversion from the transcendental equation (2.2) to a quadratic equation for T. The analytical form of the solution of (2.2) makes it possible to perform a rougher joining of the subsonic and supersonic branches of the solution and, by reducing H_0 to a small part of the calculation after the joining, to avoid the

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*Equation (1.7) should be used with caution, since it can give a large error for strongly anharmonic oscillators [2]; in such cases it is reasonable to set $\varkappa_r = 1$ as an approximation.

appearance of imaginary roots for T in this case. This considerably decreases the number of iterations in the selection of G without detriment to the accuracy of the solution.

As the starting data we use T_s, ρ_s, n_{si}, and ε_{sk} in the subsonic region. The calculating scheme is the following: 1) a step in x, solution of subsystem II with the values of n_i and ε_k in the preceding step; 2) solution of subsystem I with the T and ρ obtained; 3) successive recalculation and comparison with the available values of the parameters, then, depending on the accuracy of the result obtained, either recalculation or a new step in x, etc The choice of the size of the step in x is made automatically as a function of the total number of iterations in each step.

3. KINETIC SCHEME OF CALCULATION

The program compiled allows one to make calculations of the chemical- and vibrational-nonequilibrium flow of a gas mixture of the elemental composition H–O–C–N–inert gas. At temperatures T < 4000°K under the conditions of flow through a nozzle it is sufficient to allow for the following components for a calculation of the composition with 0.1% accuracy: CO_2, H_2O, CO, H_2, O_2, OH, N_2, NO, H, O. The chemical reactions and the channels of vibrational relaxation which are important from the aspect of the formation of a population inversion of the CO_2 vibrational levels and the effect on the flow parameters are written in accordance with the composition.

Chemical reactions:

$$CO + O + M \rightleftarrows CO_2 + M; \tag{3.1}$$

$$H + OH + M \rightleftarrows H_2O + M; \tag{3.2}$$

$$2O + M \rightleftarrows O_2 + M; \tag{3.3}$$

$$2H + M \rightleftarrows H_2 + M; \tag{3.4}$$

$$H + O + M \rightleftarrows OH + M; \tag{3.5}$$

$$O_2 + CO \rightleftarrows CO_2 + O; \tag{3.6}$$

$$O + H_2 \rightleftarrows H + OH; \tag{3.7}$$

$$O_2 + H \rightleftarrows OH + O; \tag{3.8}$$

$$H + H_2O \rightleftarrows H_2 + OH; \tag{3.9}$$

$$O + H_2O \rightleftarrows 2OH; \tag{3.10}$$

$$H + CO_2 \rightleftarrows OH + CO; \tag{3.11}$$

$$N_2 + O_2 \rightleftarrows 2NO. \tag{3.12}$$

Channels of vibrational relaxation:

$$Y_i(v_k + 1) + M \rightleftarrows Y_i(v_k) + M.\ Y_i(v_k + 1) = CO_2(01^10),$$
$$CO(1).\ NO(1).\ O_2(1),\ H_2(1),\ OH(1).\ N_2(1),\ H_2O(01^10);$$

$$CO_2\,(00^01) + M \rightleftarrows \begin{cases} CO_2\,(03^10) + M & (3.13a) \\ CO_2\,(11^10) + M; & (3.13b) \end{cases}$$

$$CO_2(00^01) + Y_i(0) \rightleftarrows CO_2(00^00) + Y_i(1),\ Y_i = N_2,\ CO;$$

$$N_2(1) + Y_i(0) \rightleftarrows N_2(0) + Y_i(1),\ Y_i = NO.\ O_2,\ CO;$$

$$CO(1) + Y_i(0) \rightleftarrows CO(0) + Y_i(1),\ Y_i = O_2,\ NO;$$

$$H_2O(01^10) + O_2(0) \rightleftarrows H_2O(00^00) + O_2(1).$$

Here M is any molecule. The rate constants of the chemical reactions are taken from [11, 12]. The experimental values of [13-22] were mainly used for the probabilities of the vibrational transitions, but for some of the processes of vibrational–translational exchange for different M they were calculated in accordance with the well-known theory of Shvarts, Slavskii, and Gertsfel'd. The relaxation channels (3.13a) and (3.13b) were combined into one with an effective exchange probability $P^{(9)}_{CO_2,M}$, which is what is usually determined in experiments [2, 23].

4. RESULTS OF CALCULATION

The results of a numerical solution of the problem, which illustrate the interaction of the chemical and vibrational nonequilibrium in the flow of a multicomponent gas mixture through a nozzle, are presented below. The flow of a mixture with the following elemental composition (in g-atom per kg of mixture) was calculated: H, 9.53; O, 15.76; N, 47.32; C, 6.31; the flow passed through a plane wedge-shaped nozzle with aperture angles of 60° for the converging part and 30° for the diverging part, with a critical section in the form of a slot with a height $h = 0.55$ cm and a width of 40 cm, rounded in the throat along a circle 0.2 cm in radius, and changing into a plane-parallel channel with a height $a = 1.6$ cm. The parameters of the stagnation mixture were $p_0 = 10$ atm and $T_0 = 3000°K$ with the equilibrium concentrations of CO_2, N_2, H_2O, CO, OH, O_2, H_2, NO, H, and O being in the ratio of 1:6.97:1.16:0.88:0.17:0.15:0.14:0.12:0.06:0.04, respectively. The starting conditions were in equilibrium and $T_S = 2990°K$. In the calculations with allowance for the interaction of the vibrational and chemical kinetics it was assumed that $\beta_{r1} = 1$, $\beta_{r2} = 0$, and $\beta_{r3} = 1$ for CO_2* while the other β_{ri} are equal to each other.

The ratios $n_i/(n_i)_0$ of concentrations of the components to their values in the reservoir as a function of x in the process of flow of the mixture with vibrational and chemical nonequilibrium are presented in Fig. 1 [1) H; 2) O_2; 3) H_2O; 4) CO_2; 5) CO; 6) H_2; 7) O; 8) OH]. The solid curves correspond to calculation with allowance for the interaction of the vibrations and the chemistry while the dashed curves correspond to calculation without it. As one would expect (solid curves), the strongest change in composition takes place in the transonic region of flow ($x \sim 0$) and then rapid freezing in of the recombination reactions (3.1)-(3.5) occurs [reaction (3.1) is already frozen in in the subsonic region at $x \simeq -0.05$; $x = 0$ in the throat]. The fast exchange reactions (3.6)-(3.11) continue to proceed intensively in the supersonic region also, which is indicated by the behavior of the concentrations of the components OH, H, and O.

A comparison of the quantities R_r and R_r' showed that during the entire expansion processes these reactions go mainly in the exothermic directions (3.6'), (3.8")-(3.12"),† while under the nonequilibrium conditions in the supersonic region the dissociation reactions (3.1")-(3.5"), the rates of which are comparable with the rates of the exchange reactions [see (2.7)], begin to play an important role.

The difference between the dashed and solid curves for O is due to the effect of the vibrational nonequilibrium on the rates of the reactions (3.1")-(3.5") (the dashed curves which differ from the corresponding solid curves by less than 1% are not shown in Fig. 1). But on the whole the effect of the interaction of the chemistry and the vibrations on the chemical composition is unimportant, since the O content in the mixture is small.

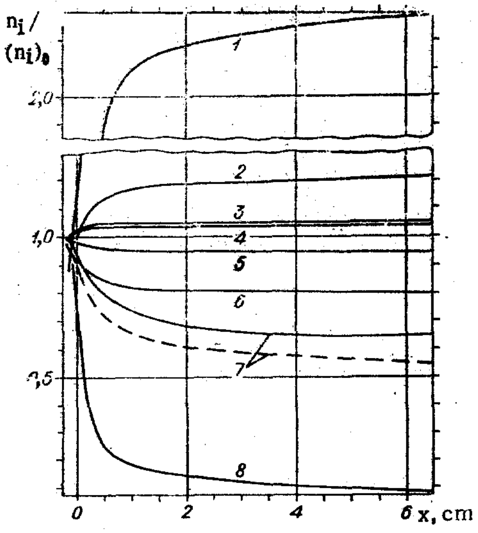

Fig. 1

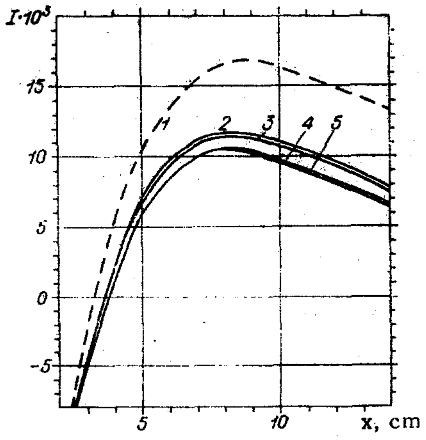

Fig. 2

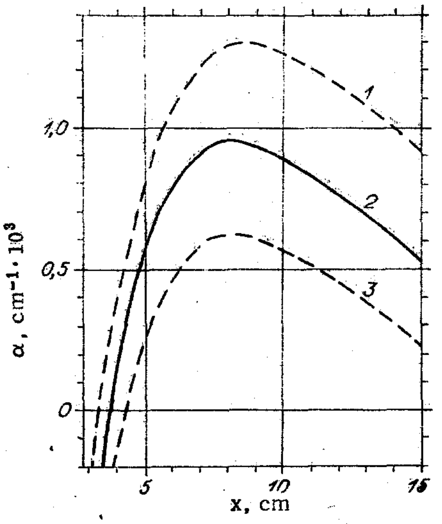

Fig. 3

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*Here and later the indices 1, 2, and 3 pertain to the symmetric, deformation, and asymmetric modes of CO_2, respectively.

†A reaction number with two primes indicates a reaction direction from right to left while a number with one prime indicates a direction from left to right.

The interaction of the chemical reactions and the processes of vibrational energy exchange is shown in Fig. 2, where the dependence of the inversion $I(x) = [n_{CO_2}(001) - n_{CO_2}(100)]/n_{CO_2}$ is presented for calculations made under different assumptions concerning the chemical and vibrational kinetics. Curve 2 corresponds to the calculation discussed above with allowance for the interaction of the chemical and vibrational nonequilibrium, the dashed curve 1 corresponds to a calculation of only the vibrational relaxation with a constant composition, and 3 corresponds to the absence of an effect of the vibrational nonequilibrium on the rates of the chemical reactions. Neglect of the chemical reactions leads to considerable overstatement (by 40% at $I \simeq I_{max}$) of the population inversion. Curve 4 represents the calculation made without allowance for the interaction of the chemical and vibrational nonequilibrium. The difference between curves 1 and 4 (56% at $I \simeq I_{max}$) is due to the fact that the chemical reactions decrease the degree of dissociation of the mixture; the latter leads to "milder" gasdynamics (the effective adiabatic index decreases) and, consequently, to a decrease in the vibrational nonequilibrium as a whole. The difference between curves 2 and 4 comprises 10% at $I \simeq I_{max}$ and is due to the "pumping" of energy into the vibrational modes owing to the chemical reaction.

The effect of the chemical reactions on the vibrational relaxation is dominant in the interaction of the chemical and vibrational nonequilibrium. This is indicated by the position of curve 3 (in contrast to the calculation for curve 2, here all $\varkappa_r = 1$), which is considerably closer to curve 2 than to curve 4. If one excludes the effect of the exchange reactions (3.6)-(3.12) in Eqs. (1.2) and sets all $\varkappa_r = 1$ (a similar model was used in [4]) then the calculation gives curve 5 for $I(x)$. A comparison of curves 3, 4, and 5 shows that the exchange reactions (3.6)-(3.12), which lead to an increase in I on the whole, principally affect the processes of vibrational relaxation.

From the foregoing it follows, for example, that the variation in the CO_2 concentration in the supersonic region of flow is described within the framework of the adopted model by the following mechanism: formation of CO_2 molecules in the exchange reaction (3.11") with subsequent partial disappearance in the dissociation reaction (3.1"). In this case the effect of the reactions (3.6') and (3.6") is negligibly small (this is indicated by the quantities R_6 and R_6'); the reactions (3.12') and (3.12") are also very slow.

The coefficient of optical amplification α, calculated from an equation presented in [24], is a GDL characteristic which is often used and is measured with high accuracy; the value of the Einstein coefficient for the spontaneous transition $CO_2(001) \rightarrow CO_2(100)$ is taken from [25]. The dependence $\alpha(x)$ is presented in Fig. 3. Curves 1 and 2 (T_s = 2990°K) are obtained from the same calculations as curves 1 and 2 in Fig. 2.

As already mentioned above, the chemical reactions are most intensive in the near-critical region of flow; in addition, both chemical and vibrational nonequilibria occur even in the subsonic region ($\approx$100°). Therefore, for correct allowance for chemical and vibrational nonequilibria in the flow through the nozzle the calculation must start from the subsonic region and the correct choice of the starting point of the calculation is important. The latter is illustrated by the dashed curve 3, obtained from a complete kinetic calculation like the calculation for curve 2 but with T_s = 2900°K in contrast to curve 2, where T_s = 2990°K. Their difference (35% at $\alpha \simeq \alpha_{max}$) characterizes the effect of the chemical and vibrational nonequilibria which develop in the subsonic region (in these calculations the critical temperature is ≃2600°K) on the quantity α.

One should expect that the effect of the chemical nonequilibrium will decrease with a decrease in T_0. A calculation made for a mixture of the same elemental composition as above but with T_0 = 2500°K showed that under these conditions the effect of the chemical reactions on the quantity α is unimportant (no more than 5%) and it can be neglected.

Let us consider the question of the effect of the vibrational nonequilibrium on the flow parameters, i.e., the question of at what values of τ_f the use of the assumption (0.1) begins to introduce an error into the calculation of T, ρ, and v. To clarify this we made calculations for different nozzles; in doing this we varied only the quantities h and α among the parameters of the nozzle described above. A comparison of the results of complete kinetic calculations with calculations in which only the chemical nonequilibrium was taken into account (all $T_k = T$) showed that the effect of vibrational nonequilibrium on the flow parameters becomes important for nozzles with $\bar{\tau}_f \lesssim 10^{-6}$ sec, where $\bar{\tau}_f$ is the average characteristic time of the flow. For example, for a nozzle with $h = 0.55 \cdot 10^{-1}$ cm and $\tau_f = 0.7 \cdot 10^{-6}$ sec the allowance for vibrational nonequilibrium changes T, ρ, and v by 5.6, 5.3, and 1%, respectively, when p = 1 atm, while for a nozzle with h = 0.55 cm and $\tau_f = 0.6 \cdot 10^{-5}$ sec the corresponding values are 1.3, 1.2, and 0.3%.

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THEORY OF A STEADY CO LASER

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The kinetic equations describing the operation of a CO laser, which is one of the most promising in terms of efficiency and specific characteristics, consist of a nonlinear system of high order (30-60). The numerical studies which have been made of the parametric functions of the generation power are inadequate for the analysis of experimental data and the design of new systems. In the present report we propose a simple model of a CO laser which makes it possible to find the power and the generation spectrum as functions of the parameters of the instrument.

An approximate analytical theory of the distribution of diatomic molecules by vibrational levels under the conditions of strong separation of the effective vibrational temperature T_1 from the gas temperature T was constructed in [1, 2]. The condition of applicability of the resonance approximation used in [1, 2] has the form

$$\exp(-\delta_{VV}v^*) \ll C\frac{6\Delta E}{T\delta_{VV}^3},$$

where $C = (v^* + 1)f(0)\exp[-(\Delta E/T)(v^*)^2 - 1/2]$ [$f(0)$ is the fraction of molecules in the ground state]; ΔE is the anharmonicity of a molecule; v^* is a number corresponding to the Treanor minimum [3]; δ_{VV} is a number which depends on the gas temperature and characterizes the rate of exchange with the resonance defect [2].

Allowance for radiative transitions within the framework of [1, 2] gives the equation

$$\frac{3Q_{10}}{\delta_{VV}^3}\frac{d}{dv}\left[(v+1)^2 f^2\left(\frac{2\Delta E}{T} - \frac{d^2\ln f}{dv^2}\right)\right] + P_{10}(v+1)f\exp(\delta_{VT}v) + \\ + A_{10}(v+1)f + \frac{I_v}{\hbar\omega_v}\sigma(v)\left[\gamma_v f + \frac{df}{dv}\right] = 0, \tag{1}$$

where P_{10} and A_{10} are the probabilities of the collisional and radiative transitions (1 → 0); Q_{10} is the probability of exchange in a collision of CO molecules; I_V is the light intensity in the transition $v + 1 \rightarrow v$; $\hbar\omega_V = E_1 - 2\Delta Ev$; $\gamma_V = 1 - \exp[-2B_V(j_V + 1)/T]$; B_V is the rotational constant; j_V is the rotational quantum number at which generation in the band $v + 1 \rightarrow v$ takes place; $\sigma(v)$ is the cross section for stimulated emission. The remaining notation is as in [2].

The independence of T_1 from the presence of generation follows from Eq. (1). This conclusion is confirmed by the numerical calculations of [4]. The loss rate is determined by the quantum flux formed in the region of the Treanor minimum by V–V processes and depends only on T_1 and the gas temperature. The connection between T_1 and T, if the pumping is concentrated in the lower levels, is found from the equation

$$q = \eta_v\frac{jE}{N_{CO}E_1} = \frac{6Q_{10}}{\delta_{VV}^3}\frac{\Delta E}{T}C^2(T_1),$$

where $q \ll (6Q_{10}/\delta_{VV}^3)(\Delta E/T)^3$. Here jE is the power released in the discharge; η_V is the portion expended on the excitation of vibrations; N_{CO} is the density of CO molecules.

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