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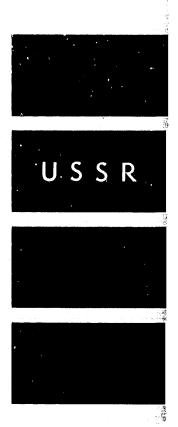
25 JUNE 1979

PHYSICS OF COMBUSTION AND EXPLOSION (FOUO 35/79)

1 OF 1

JPRS L/8540 25 June 1979

TRANSLATIONS ON USSR SCIENCE AND TECHNOLOGY
PHYSICAL SCIENCES AND TECHNOLOGY
(FOUO 35/79)
PHYSICS OF COMBUSTION AND EXPLOSION



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TRANSLATIONS ON USSR SCIENCE AND TECHNOLOGY PHYSICAL SCIENCES AND TECHNOLOGY

(FOUO 35/79)

PHYSICS OF COMBUSTION AND EXPLOSION

Moscow FIZIKA GORENIYA I VZRYVA in Russian Vol 15, No. 1, Jan-Feb 79 pp 84-102, 119-125

[Selected articles from journal edited by L.S. Kravchenko, Izdatel'stvo "Nauka", 1625 copies, 128 pages]

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PHYSICS

THE FLOW FIELD AND GAINS IN THE RESONATOR CAVITY OF A GAS DYNAMIC LASER USING KEROSENE COMBUSTION COMBUSTION PRODUCTS. A TWO-DIMENSIONAL CALCULATION AND EXPERIMENTAL COMPARISON

Novosibirsk FIZIKA GORENIYA I VZRYVA in Russian Vol 15 No 1, Jan-Feb 79 pp 84-89

[Article by M.G. Ktalkherman, V.A. Levin, V.M. Malkov and Yu.V. Tunik, Moscow, Novosibirsk, manuscript received 28 Mar 78]

[Text] A purely experimental search for the optimum operational conditions of a GDL [gas dynamic laser] and the shape of its nozzle is too labor intensive, and for this reason, numerical modeling of the physical processes in high power laser systems acquires considerable significance in their design.

The solution of problems of the outflow of the relaxing mixture of gases from a GDL nozzle is usually managed using one-dimensional approximations [1], which most often are in qualitative agreement with experimental findings. The actual picture of the flow in a resonator cavity is characterized by the presence of viscous trails and shock waves, which exert a considerable influence on the amplifying properties of the medium [2]. Under these conditions, the use of one-dimensional calculations yields a too approximate picture of the flow, since the parameters transverse to the flow can vary significantly. Both experiments and calculations indicate this.

A two-dimensional calculation procedure was employed in [3] for the flow of a relaxing mixture, which permits distinguishing the shock waves in the nozzle. For a correct comparison of this procedure with experiments, data are needed on the flow structure, since in nozzles with a point of inflection and large initial aperture angles, which are usually employed in GDL's, the flow can be far from one-dimensional and the appearance of shocks is possible. Such information is usually lacking in papers dealing with the measurements of gain. We will also note that the divergence of the numerical results from experimental ones can be due to the indeterminancy in the constants for relaxation processes [4].

A comparison of two-dimensional calculations of the flow fields and the gains in a constant cross-section channel adjacent to a nozzle is presented in this

paper. The structure of the flow in the channel was characterized by the presence of shock waves. The agreement between the mathematical model and the actual processes under these conditions is subjected to a serious check.

At the present time, GDL's using the combustion products of liquid hydro-carbonfuels are extremely promising [5 - 7], because of the accessibility of the fuel and the relative simplicity in obtaining large mass rates of flow of the active lasing media with acceptable amplification properties. The amplification properties of kersene combustion products, flowing out from a radius nozzle, and the main aerodynamic characteristics of the flow in the channel adjacent to it were computed and measured in this work.

Radius nozzles - nozzles with an inflection point - where the supersonic portion of the nozzles is profiled as the arc of a circle, are of interest because of their technological qualities.

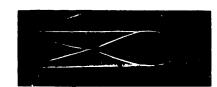


Figure 1. A shadow photograph of the flow in the channel.

The basic geometric parameters of the nozzle are: the critical cross-section height $h^*=0.7$ mm, the output cross-section, H=20 mm. There is a small band 0.2 mm wide in the critical region, which by means of rounding off to a radius of 0.5 mm was mated to the wedge-shaped subsonic section (the half-angle of the wedge is 60°). The radius of the supersonic section

profile was equal to 37.5 mm. The initial half-angle of the nozzle aperture was $\theta_{\rm H}$ = 42°. The nozzle was smoothly mated to the constant cross-section channel with a height of 20 mm. The width of the channel in the sounding direction was 180 mm.

A detailed description of the setup and procedure for the measurements were given in [6]. A slight difference in the measurement circuit, related to the specific features of the given experiments, consisted in the fact that the beam of the sounding laser was collimated, and a diaphragm stop 1.5--2 mm in diameter was placed ahead of the input window. Any point in the channel could be probed. The trials were conducted at a braking temperature of $T_0 = 1,000-1,600\,^{\circ}$ K and a pressure in the precombustion chamber of p_{φ} [t_f] = 20 atm.

A special working section, consisting of a similar nozzle with a 110 mm long channel was fabricated for the aerodynamic measurements (in cold air). The width of the working section was 80 mm, and the side walls were made of optical glass. The visualization of the flow was realized using a direct shadow method. During the measurement of the static pressures, the glass in the side walls was replaced by drain inserts. There were also drain holes in the shaped portion of the nozzle and in the center of the upper wall of the channel.

A photograph of the flow picture obtained in trials with cold air is shown in Figure 1. The structure of the flow can be clearly seen. The shocks intersect at a distance of $^{\rm c}$ 56 mm from the critical cross-section (the numbers along the bottom of the channel give an idea of the scale). The configuration of the shock waves found by calculation is shown in Figure 2. As can be seen, the agreement is practically total.

The distribution of the static pressure p/pf at the side wall (y = 0) and the shaped wall of the working section is shown in Figure 3, where x is the distance from the critical section. The observed pressure peak at the shaped wall corresponds to the point of shock departure. Thereafter, the pressure falls off, and at a distance of 75-80 mm approaches a value of $p/p_f=1.5\cdot 10^{-3}$, which was found from one-dimensional calculations. The pressure at the side wall reaches a minimum in the output cross-section of the nozzle $(p_{min}/p_f=1.5\cdot 10^{-3})$. The pressure increase at the side wall on the downstream side is due to shock waves, where $p_{max}/p_{min}=3$. A doubling of the pressure in the precombustion chamber (from 21 to 41 atm) does not change the distribution of p/p_f , something which indicates the insignificant influence of viscous effects under the conditions of the experiment (the Reynolds number, computed from the parameters of the flow in the critical cross-section and its height was $Re_{h\pi}=3.8\cdot 10^5$ at $p_f=30$ atm).

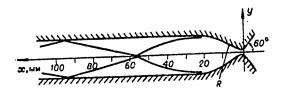


Figure 2. The configuration of the shock waves in the channel (calculated).

Pressure profiles were obtained in several channel cross-sections using probes. The distribution of p_0/p_f over the height of the channel is shown in Figure 3 (p_0' is the pressure behind a forward shock). The point of shock passage and the perturbation it induces, by the amount p_0'/p_f , can be clearly seen. The static pressure profiles were measured at these same cross-sections and several of them are given below. Local Mach numbers were determined from the quantity p/p_0' . In the central portion of the flow at the outlet from the nozzle, M = 4.6, and at the section x = 100 mm, M = 4.1. The static pressure at these sections differs by almost a factor of two. We will note that the one-dimensional calculation yields M = 5.1 (for an adiabatic exponent of $\kappa = 1.4$).

The previously developed procedure of [3], the use of which makes it possible to single out the shock waves arising in the flow, and which brings the

mathematical model close to actual flows, was employed in the two-dimensional calculations of the flow of a relaxing gas in a nozzle. The relaxation equations were solved simultaneously with the equations of motion, continuity and energy. The solution was based on a difference scheme using the through count procedure for supersonic flows. The details of the numerical calculations can be found in [3, 8].

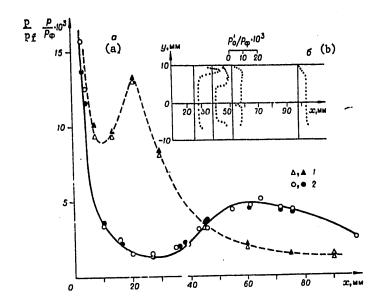


Figure 3. The pressure distribution at the walls (a) and the quantities p_0^\prime/p_f over the height of the channel (b) (the dark dots are for $p_f=21$ atm, and the light ones are for $p_f=41$ atm).

Key: 1. Profiled wall;
2. Side wall.

The results of recent work on the determination of relaxation transition constants, a review of which was pulbished in [9], were employed to describe the oscillatory exchange processes. The constants employed in the work are given in Table 1. The composition of the kerosene combustion products in air are presented in Table 2.

Table 1

Process n'ponecc	м	Qij¹ w v _{ij} , atm.c & atmosec				
$CO_2(v_1+v_2)+M \rightleftharpoons CO_2+M$	CO2	$\lg \tau = 17,42 \times x - 7,85$				
	N ₂	15,55×x—8,06				
(VT)	02	15,55×x-8,06				
	H ₂ O	τ=3.10-9				
N5+M≠N2+M	CO2	$\lg \tau = 104 \times x - 11,2$				
,	N ₂	99,5×x-10,76				
(VT)	O ₂	95,5×x-10,76				
	H ₂ O	36,8× <i>x</i> —9,812				
$CO_2(v_3)+M \rightleftharpoons CO_2(v_1+v_2)+M$	CO ₂	$\ln \sigma = -9,456 + 218,23 \times x -$				
Q=8.106		$-1687,7 \times x^2 + 3909,3 \times x^3$				
(VT)	N ₂	$-15,457+424,03\times x-3852,7\times \times x^2+10672,2\times x^3$				
•	Og	-15,457+424,03×x				
		$-3852,7 \times x^{2} + 10672,2 \times x^{3}$				
	H ₂ O	1g Q=5,62+11,2×x				
$CO_3(v_3)+M \stackrel{\sim}{=} CO_2+M^v$ $(i) \leftarrow (VV) \rightarrow (j)$	N ₂	$\log Q = 7,42 - 1,65 \cdot 10^{-3} \cdot T + 5,7 \cdot 10^{-7} \cdot T^{2}$				
Note: $x=r^{-1/3}$.	-					

The following oscillatory energy exchange processes were taken into account:

$$CO_2(v_1+v_2)+M \Rightarrow CO_2+M,$$

 $N_2^{\circ}+M \Rightarrow N_2+M,$
 $CO_2(v_3)+M \Rightarrow CO_2(v_1+v_2)+M,$
 $CO_2(v_3)+M \Rightarrow CO_2+M^{\circ}.$

In accordance with the procedure proposed in [16], nonequilibrium oscillatory temperatures were introduced to describe the kinetic processes: $T_1 = T_2$ are the symmetric and deformational modes of CO₂, T_3 is the antisymmetric mode of CO₂, and T_4 is for nitrogen. The equations for the $e_1 = [\exp{(\theta_1/T_1)} - 1]^{-1}$ have the form:

$$\begin{split} \frac{de_2}{dt} &= \lambda_2 \Big[\Phi_{23} - \left(e_2 - e_2^0 \right) \frac{\rho}{\tau_1} \Big], \\ \frac{de_3}{dt} &= - \Phi_{28} + \xi_2 \Phi_{31}, \end{split}$$

$$\frac{de_4}{dt} = \xi_1 \Phi_{34} - (e_4 - e_4^0) \frac{p}{\tau_2},$$

$$e_1 = e_2^2 (2e_2 + 1), \quad \lambda_2 = (1 + 2e_2)^2 / (1 + 6e_2 + 6e_2^2).$$

Here, p is the pressure, T is the temperature, e_1^0 is the value of e_1 at $T_1 = T$, ξ_1 is the molar concentration of CO_2 , ξ_2 is for N_2 , ξ_3 is for O_2 and ξ_4 is for H_2O_3 ;

$$\Phi_{ij} = PQ_{ij}\phi_{ij};$$

$$\phi_{ij} = \begin{cases} e_{j} (e_{i} + 1)^{3} - \exp\left[(3\theta_{i} - \theta_{j})/T\right] (e_{j} + 1) e_{i}^{3} & (i, j = 2,3) \\ e_{j} (e_{i} + 1) \exp\left[(\theta_{j} - \theta_{i})/T\right] - e_{i} (e_{j} + 1) & (i, j = 1,4); \end{cases}$$

 θ_{ij} are the probabilities of the exchange (V-V)-processes; the relaxation times τ_i are computed from the relationships $\tau_i^{-1} = \sum\limits_{j=1}^L \xi_j \tau_{ij}^{-1}; \quad \theta_i$ are the characteristic temperatures of the corresponding oscillation modes.

The following characteristic sections were selected for detailed calculations and measurements: 37, 56 and 104 mm. In the first, the parameters of the flow in the central portion are close to the parameters at the outlet from the nozzle, the second is located in the intersection region of the shocks, while the third is located in the region where the shocks are reflected from the channel walls (see Figure 1).

Table 2

Т•. Қ	CO1	H ₂ O	N,	0,		
1200 1400	0,05 0,0625	0,045 0,055 0,0675 0,08	0,765 0,765 0,76 0,755	0,15 0,13 0,11 0,09		

The comparison results are shown in Figure 4, where the distribution of the gain $\,k\,$ over the height of the channel is given, as well as the static pressure p/p_f , the flow temperature T and the quantities T_2 , T_3 and T_4 at T_0 = 1,400° K and p_f = 20 atm. The good qualitative and altogether satisfactory quantitative agreement of the calculated and measured values can be cited. When passing through a shock, the quantities $\,k$, $\,p$, T and $\,T_2$ change sharply. The observed

decrease in the gain is due to the increase in the static pressure and the flow temperature, which lead to an intensification of the relaxation processes, and in the final analysis, to an increase in the population of the lower lasing level. A reduction in k in this case is extremely important. Thus, on the channel axis (y=0), according to the measurements, the gain at the 104~mm section is 2.5 times less than at the 37~mm section.

The influence of shock waves on the amplifying properties of the medium differs throughout the entire range of change in the parameters. Figure 5

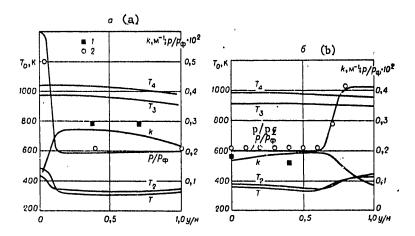


Figure 4. Profiles of the temperatures, pressure and gains. a) x = 56 mm, $T_0 = 1,400^{\circ}$ K; b) x = 104 mm, $T_0 = 1,400^{\circ}$ K;

b)
$$x = 104 \text{ mm}$$
, $T_0 = 1,400^{\circ} \text{ K}$;

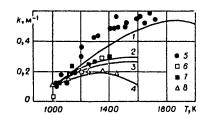


Figure 5. A comparison of the experimental and calculated gains as a function of temperature (1-4 are calculated, 5-8 are experimental).

Key: 1,5.
$$x = 37 \text{ mm}$$
, $y = 0$;
2,6. $x = 56 \text{ mm}$, $y = 4 \text{ mm}$;
3,7. $x = 56 \text{ mm}$, $y = 7 \text{ mm}$;
4,8. $x = 104 \text{ mm}$, $y = 0$.

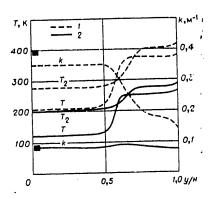


Figure 6. Temperature profiles and gains at the section x = 37 mm.

Key: 1.
$$T_0 = 1,400^{\circ}$$
 K;
2. $T_0 = 1,000^{\circ}$ K.

illustrates this, where the function $k(T_0)$ is plotted at several points in the selected cross-section. It can be seen that with an increase in To, the influence of shock waves increases, but it is insignificant (for the given nozzle) up to $T_0 \simeq 1,150^\circ$ K. This is related to the fact that an increase in the forward temperature and T_2 following a shock up to a value of $\simeq 300^\circ$ K does not lead to a marked rise in the population of the lower lasing level. The graph in Figure 6 is characteristic in this sense. In both cases, the change in the temperature in a shock is identical, but for $T_0 = 1,000^{\circ}$ K, the forward temperature following a shock is low and the change in the gain is insignificant. For nozzles with a large ratio of (H/h*), the value of To, up to which shock waves have a slight influence on the size of k, will apparantly increase (for the close pressures in the resonator).

In conclusion, the authors would like to thank N.A. Ruban and Ya.I. Kharitonova for assisting in the conduct of the experiment and the processing of the results.

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PHYSICS

A NUMERICAL ANALYSIS OF THE VIBRATIONAL MODE OF A CW CHEMICAL HF LASER

Novosibirsk FIZIKA GORENIYA I VZRYVA in Russian Vol 15 No 1, Jan-Feb 79 pp 89-97

[Article by A.V. Lavrov, V.A. Pospelov, A.V. Fedotov and M.L. Shur, Leningrad, manuscript received 23 Jan 78]

[Text] The development of Polanyi's concept [1] of the creation of an inverted medium in the process of exothermal chemical reactions leads to the design of supersonic chemical diffusion type lasers [2, 3]. At the present time, it can be considered as an established fact that one of the most promising systems of this type is the laser using the hydrogen flouride HF molecule. An HF laser is treated in this paper, in which separate feeds of the fuel (molecular hydrogen) and the oxidant with a diluting agent (partially or completely dissociated fluorine and helium) in a system of plane parallel streams (Figure 1) are used to produce a medium with an inverted population. The vibrational excited molecules of hydrogen fluoride are formed in the resonator when the streams of the fuel and the oxidant mix as a result of pumping:

$$F+H_2 \longrightarrow HF(v)+H+Q_1, \quad v \leq 3,$$

$$F_2+H \longrightarrow HF(v)+F+Q_2 \quad v \leq 8.$$
(1)

Here $\,v\,$ is the number of the vibrational level of the excited molecule; ${\rm Q}_1$ and ${\rm Q}_2$ are the thermal effects of the reaction,

A characteristic feature of the flow in the resonator of a chemical laser consists in the mutual influence of the gas dynamic processes, the fast chemical reactions and the coherent radiation fields. A consequence of this is that a rather complete concept of laser operation can be obtained only with a numerical solution of the gas dynamic equations which describe the flow in the resonator.

At the present time, there are examples of the calculations of CW chemical lasers based on boundary layer equations in the literature [4 - 6], however, a detailed parametric study of laser operation in the vibrational mode has been

carried out only within the framework of a one-dimensional model of the instantaneous intermixing [7] and a quasi-one-dimensional model of the flame front [8]. In this paper, a parametric analysis is made of the oscillation mode on the basis of boundary layer equations; the results are compared with the data of paper [8].

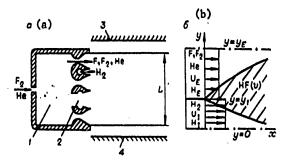


Figure 1. Basic schematic of a supersonic CW chemical HF laser.

Key: 1. Precombustion chamber;

2. Nozzle unit;

3,4. Reflectors with reflection factors of rL and ro.

The Kinetic Scheme and the Calculation of the Small Signal Gain

The total number of chemical reactions for the mixture considered here is extremely large. The following reactions are considered in this paper: pumping reactions (1) and (2), V-V exchange reactions between the HF (v) molecules, V-P deactivation reactions of the HF (v) molecules with different mixture components, as well as dissociation (recombination) reactions. The total aggregate of the processes being considered and the corresponding rate constants are given in [8].

It was assumed in calculating the small signal gain that the contour of a line is determined by the doppler widening. It was likewise assumed that at each vibrational level, equilibrium distribution of the HF molecules occurs with respect to the rotational sublevels. In this case, oscillation is realized in the P-branch of the vibrational-rotational transitions $(v+1, J-1) \rightarrow (v, J)$ for the case of a value of a rotational quantum number J corresponding to the maximum gain. The expression for the gain $\alpha_{v,J}$ has the form:

 $\alpha_{\bullet, j} = \rho[F_{2, \bullet, j}(T)c_{\bullet+1} - F_{1, \bullet, j}(T)c_{\bullet}].$ (3)

Here ρ is the density; c_v is the relative HF (v) mass concentration; T is the temperature; and the expressions for $F_{2,v,J}$ and $F_{1,v,J}$ are given in [8].

10

the Prandtl number; NA is Avogadro's number; h is Planck's constant; MHF is the molecular weight of the HF molecules; R is the universal gas constant; M is the molecular weight of the mixture. System (4) - (9) was written with the following assumptions: the Lewis number is Lei = 1, the Prandtl number is P_r = const, (a value Pr = 0.17 was used in the numerical calculations).

The boundary conditions for the given system of equations have the form:

$$x=0, \ 0 \le y \le y_1, \ f = f_1;$$

 $x=0, \ y_1 < y \le y_2, \ f = f_2;$
 $x>0, \ y=0, \ \partial f / \partial y = 0, \ v=0;$
 $x>0, \ y=y_2, \ \partial f / \partial y = 0.$ (10)

Here f is any of the functions of u, H or ci. The subscripts I and E correspond to the initial values of the parameters in the oxidant and fuel flows.

It is easy to see that system (4) - (9) is not a closed one, since included in it are unknown pressure gradients and radiation intensities (dp/dx and Ii are functions only of x). The condition for the preservation of the mass rate of flow between the axes of symmetry of the two adjacent streams was employed to close the system:

$$\int_{1}^{\nu_{E}} \rho u dy = \text{const}$$
 (11)

as well as the condition for quasisteady-state oscillation (i.e., the condition that over the extent of the vibrational region the integral gain factors of the radiating transitions are equal to the threshold value, which is defined in terms of the reflection factors of the resonator reflectors r_0 and r_I and the length of the optical path):

$$\int_{0}^{y_{E}} \alpha_{i} dy = -\frac{1}{2} \frac{\ln(r_{e}r_{L})}{2y_{E}N_{cn}}.$$
 (12)

here, N_{CA} is the overall number of mixing layers.

The solution method. The problem was solved in Mises variables x and ψ [10], where ψ is a function of the current, defined in the usual manner. The system of equations (4) - (8), the boundary conditions (10), and the integral conditions (11) and (12), assume the following form with the transition to Mises variables: $\frac{\partial u}{\partial x} = \left(\frac{\partial u}{\partial x}\right) - \frac{1}{\rho u} \frac{\partial \rho}{\partial x}$:

$$\frac{\partial x}{\partial x} = \left(\frac{\partial x}{\partial x}\right)_{\bullet} - \frac{\partial u}{\partial x} = \frac{\partial x}{\partial x}.$$
(13)

$$\frac{\partial H}{\partial x} = \left(\frac{\partial H}{\partial x}\right)_{0} - \frac{1}{\rho u} \sum_{i=1}^{N_{1}-1} \alpha_{i} I_{i}; \tag{14}$$

$$\frac{\partial c_l}{\partial x} = \left(\frac{\partial c_l}{\partial x}\right)_0 + \frac{M_{HF}}{h N_A} \frac{1}{\rho u} \left(\frac{\alpha_i l_i}{v_l} - \frac{\alpha_{i-1} l_{i-1}}{v_{i-1}}\right), \quad l = 1, \dots, N_1; \tag{15}$$

We will note that a simplified system of indexing the transition parameters $(v + 1. J - 1) \rightarrow (v, J)$ is used in the following. Thus, for example, for the gain $\alpha_{V,J}$, the radiation frequency $\nu_{V,J}$ and the radiation intensity $I_{V,J}$, the symbols α_{1} , ν_{J} and I_{1} are used respectively, where i=v+1.

The formulation of the problem. Experimental studies [9] have shown that when realizing the calculated mode for the outflow of the fuel and the oxidant from nozzles, and for the case of a sufficiently low pressure in the resonator, there are no shock waves, and within the limits of the oscillation zone there is a laminar mixing mode. For this reason, the following laminar boundary layer equations are employed in this paper to describe the flow in the region of the resonator bounded by the axes of symmetry of the two adjacent flows, where these equations include terms which take into account the enrgy transfer and the mutual transformation of the vibrational-excited HF (v) molecules with the action of the radiation [4]:

The continuity equation:

$$\partial \rho u/\partial x + \partial \rho v/\partial y = 0; \tag{4}$$

The equation of motion projected onto the x axis:

$$\rho u \cdot \partial u / \partial x + \rho v \cdot \partial u / \partial y = -d\rho / \partial x + \partial / \partial y (\mu \cdot \partial u / \partial y); \tag{5}$$

The energy equation:

$$\rho u \frac{\partial H}{\partial x} + \rho v \frac{\partial H}{\partial y} = \frac{\partial}{\partial y} \left\{ \frac{\mu}{Pr} \left[\frac{\partial H}{\partial y} + (Pr - 1) u \frac{\partial u}{\partial y} \right] \right\} - \sum_{i=1}^{N_1 - 1} \alpha_i I_i; \tag{6}$$

The equation for the diffusion of the vibrational excited HF molecules:
$$\rho u \frac{\partial c_l}{\partial x} + \rho v \frac{\partial c_l}{\partial y} = \frac{\partial}{\partial y} \left(\frac{\mu}{\Pr} \frac{\partial c_l}{\partial y} \right) + \dot{w}_i + \frac{M_{HF}}{\hbar N_A} \left(\frac{\alpha_i l_i}{v_i} - \frac{\alpha_{i-1} l_{i-1}}{v_{i-1}} \right), \qquad i = 1, \dots, N_1; \tag{7}$$

The equation for the diffusion of the remaining component (H, H2, F, F2, He):

$$\rho u \cdot \partial c_i / \partial x + \rho v \cdot \partial c_i / \partial y = \partial / \partial y \cdot (\mu / \Pr \cdot \partial c_i / \partial y) + \dot{w}_i, \quad N_1 < i \le N.$$
 (8)

It is necessary to add the following equation of state to these equations:

$$p/p = RT/M. (9)$$

Here x and y are Cartesian coordinates (see Figure 1b); u and v are longitudinal and transverse velocity components; μ is the coefficient of viscosity; c_1 is the relative mass concentration of the i-th component; $\dot{\mathbf{w}}_1$ is the mass rate of formation of the 1-th component as a result of the chemical reactions; H is the total enthalpy of the mixture (H = $\sum_{i=1}^{n} c_i h_i + u^2/2$, $\int c_{pi}dT \div h_i^0$, where h_1^0 is the enthalpy of formation, while \overline{c}_{pi}^0 is the specific heat capacity of the i-ch component at constant pressure; P_r is

$$\frac{\partial c_1}{\partial x} \sim \left(\frac{\partial c_1}{\partial x}\right)_0, \quad N_1 < l \le N;$$

$$x = 0, \quad 0 \le \psi \le \psi, \quad f = h;$$
(16)

$$x=0, \ \forall_i < \psi < \psi_E, \ j=j_E; \tag{17}$$

x>0, $\psi=0$, $\partial f/\partial \psi=0$; x>0, $\psi=\psi_x$, $\partial f/\partial \psi=0$;

$$\int_{0}^{\Phi_{E}} \frac{d\psi}{\rho u} = \text{const} = y_{E};$$
 (18)

$$\int_{0}^{\pi} \frac{\alpha_{1}}{\rho u} d\psi = C_{0}. \tag{19}$$

The following symbols are introduced in (13) - (16):

$$\begin{split} \left(\frac{\partial u}{\partial x}\right)_{\mathbf{0}} &= \frac{\partial}{\partial \psi} \left(\mu \rho u \frac{\partial u}{\partial \psi}\right), \\ \left(\frac{\partial H}{\partial x}\right)_{\mathbf{0}} &= \frac{\partial}{\partial \psi} \left(\frac{\mu \rho u}{\Pr} \left[\frac{\partial H}{\partial \psi} + (\Pr - 1) u \frac{\partial u}{\partial \psi}\right]\right), \\ \left(\frac{\partial c_{l}}{\partial x}\right)_{\mathbf{0}} &= \frac{\partial}{\partial \psi} \left(\frac{\mu \rho u}{\Pr} \frac{\partial c_{l}}{\partial \psi}\right) + \frac{\dot{w}_{l}}{\rho u}. \end{split}$$

The following method was employed to determine the pressure gradient and the radiation intensity. We differentiate the condition for the preservation of the mass rate of flow (18) with respect to s. By varying the order of differentiation with respect to x and integrating with respect to ψ , and substituting the values of the derivatives from (13) - (16), taking (9) into account, we obtain:

 $A\frac{dp}{dx} + \sum_{i=1}^{N_i-1} B_i I_i + D = 0, \tag{20}$

where

$$A = \int_{0}^{\Psi_{E}} \frac{1}{\rho u} \left(\frac{1}{\rho} - \frac{1}{\rho u^{2}} - \frac{1}{\rho c_{p}T} \right) d\psi;$$

$$B_{t} = \int_{0}^{\Psi_{E}} \frac{\alpha_{t}}{c_{p}T} \frac{1}{\rho^{2}u^{2}} \left[1 + \frac{M_{HP}}{hN_{A}\Psi_{t}} \left(h_{t}^{0} - h_{t+1}^{0} \right) \right] d\psi;$$

$$D = \int_{0}^{\Psi_{E}} \frac{1}{\rho u} \left\{ \frac{1}{u} \left(\frac{\partial u}{\partial x} \right)_{0} - M \sum_{(1)} \frac{1}{M_{t}} \left(\frac{\partial c_{t}}{\partial x} \right)_{0} - \left(\frac{\partial u}{\partial x} \right)_{0} - \sum_{(1)} \left(\frac{\partial c_{t}}{\partial x} \right)_{0} \right\} d\psi.$$

$$- \frac{1}{c_{p}T} \left[\left(\frac{\partial H}{\partial x} \right)_{0} - \sum_{(1)} h_{t} \left(\frac{\partial c_{t}}{\partial x} \right)_{0} - u \left(\frac{\partial u}{\partial x} \right)_{0} - \sum_{(1)} \left(\frac{\partial c_{t}}{\partial x} \right)_{0} \right] d\psi.$$

In a similar fashion, taking (3) from (19) into account, one can derive: $E_{l} \frac{dp}{dx} + \sum_{i=1}^{N_{l}-1} R_{i,l} I_{j} + Q_{l} = 0. \tag{21}$

here

$$E_{l} = \int_{0}^{\sqrt{\epsilon}} \frac{1}{\rho u} \left[\frac{\lambda_{l}}{c_{p}} - \frac{\alpha_{l}}{\rho u^{2}} \right] d\eta;$$

$$Q_{i} = \int_{0}^{\Psi_{E}} \frac{1}{dt} \left\{ \left[F_{2,i} \left(\frac{\partial c_{i+1}}{\partial x} \right)_{0} - F_{1,i} \left(\frac{\partial c_{i}}{\partial x} \right)_{0} \right] + \frac{\lambda_{i}}{c_{p}} \left[\left(\frac{\partial H}{\partial x} \right)_{0} - \sum_{j=1}^{N} h_{j}^{0} \left(\frac{\partial c_{j}}{\partial x} \right)_{0} - \sum_{j=1}^{N} h_{j}^{0} \left(\frac{\partial c_{j}}{\partial x} \right)_{0} \right] - \sum_{j=1}^{N} h_{j}^{0} \left(\frac{\partial c_{j}}{\partial x} \right)_{0} - \sum_{j=1}^{N} h_{j}^{0} \left(\frac{\partial c_{j}$$

In this way, the problem of determining the pressure gradient and the radiation intensity has been reduced to the solution of a system of linear algebraic equations (20) and (21), where the number of equations depends on the number of radiative transitions. An explicit four-point finite difference scheme with a variable step with respect to ψ with iterations was employed for the numerical integration of system (13) - (16).

The basic results. A series of calculations for a CW chemical laser were performed using the procedure set forth here, where the laser was characterized by the following parameters (see [8]): an optical path length of L = 175 mm, reflection factors of the reflectors of r_0 = 0.98 and r_L = 0.85, reflector

absorption factors of a0 = a_L = 0.02, a half-he ght of the output cross-section of the "fluorine" nozzle of 2 mm, an expansion factor of the "fluorine" nozzle of 10, and the half-height of the output cross-section of the "hydrogen" nozzle was 0.5 mm.

It was assumed that for a specified temperature T_k pressure p_k and degree of dilution with an inert gas of β = y_{He}/y_{F2} (y_{He} , y_{F2} are the molar concentrations of He and F₂)in the precombustion chamber, there is equilibrium dissociation of the fluorine. Further, the mixture of molecular and atomic fluorine and helium expands in the system of supersonic nozzles, the flow in which is assumed to be uniform, nonviscous, adiabatic and the chemical reactions are considered to be quenched. The degree of dissociation of the fluorine α_g = $c_F/(c_F + c_F)$ and the flow parameters at the "fluorine" nozzle edge are shown in Figure 2 as a function of the temperature in the chamber. The velocity at the output of the "hydrogen" nozzle was set equal to 2,500 m/sec, the temperature at 200° K, while the pressure was assumed equal to the pressure at the output at the "fluorine" nozzle.

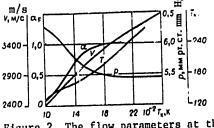


Figure 2. The flow parameters at the edge of the "fluorine" nozzle.

As a result of the calculations which were performed, curves were obtained for the main characteristics of the laser (the generation power P, the energy yield per unit of oxidant mass E, the chemical efficiency η) as a function of the parameters in the precombustion chamber. The curves for P, E and η are shown as a function of T_k in Figure 3 (P and E apply to values when T_k = 2,000° K). It is easy to see

that although the maximum efficiency corresponds to operation with complete fluorine dissociation ($T_k=2,000^\circ$ K), the specific energy yield reaches the greatest level at $T_k\simeq 1,100^\circ$ K. The power generated in this case is 1.5 times greater than the radiation power at $T_k=2,000^\circ$ K, something which is also related to the increase in the mass rate of flow of the components. Thus, for a specified geometry of the nozzle unit, one can anticipate an increase in the radiation power when making a transition to low levels of fluorine dissociation.

It can be seen from Figure 3a that the function η (T_k) is in qualitative agreement with the results of [8]. Along with this, there are rather significant quantitative differences. Thus, at a precombusion chamber temperature of 2,000° K, the efficiencies differ by 1.5 times; a low dissociation levels, the "flame front" model predicts a value of the efficiently approximately the same as at a dissociation level of α_g = 1, while in this work, the efficiency at T_k = 1,100° K falls off by 1.7 times as compared to T_k = 2,000° K.

Apparently, the quantitative difference in the results is primarily related to the presence of a considerable amount of inhomogeneity in the profiles of the gas dynamic parameters (see, for example, Figure 4), which is not taken into account in the quasi-one-dimensional model [8]. Because of the strong nonlinearity of the equations, this cannot lead to a marked difference in the results.

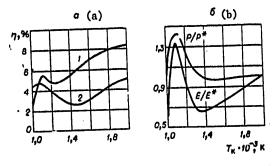


Figure 3. The efficiency (a), power and energy yield (b) as a function of the temperature in the precombustion chamber.

Key: 1. This paper; 2. Paper [8].

At high temperatures in the precombustion chamber ($\alpha_g \approx 1$), the pumping is determined only by the first term of (1), which has a high velocity. Because of this, the reaction takes place in a narrow region and the flame approximation is observed rather well (Figure 4b). At low temperatures, a considerable quantity of molecular fluorine is present in the flow. The velocity constant of the second term is considerably less than the first, and for this reason, the intense development of a chain mechanism begins only at the end of the reaction region following sufficient heating of the mixture. At this point in time, the molecular fluorine is already rather well intermixed with the hydrogen, and the reaction takes place in a broad region (Figure 4c), and therefore, the use of the flame front model at these temperatures is considerably less precise.

The laser parameters are shown in Figure 5 as a function of the reflection factor of the semitransparent reflector and the degree of inert gas dilution, β . If the efficiency increases monotonically with an increase in β , something which is related to a reduction in the part played by oscillatory deactivation, then the radiation power has a maximum at $\beta\simeq 15$. When $\beta>15$, P falls off, since an increase in the efficiency cannot compensate for a reduction in the fluorine flow rate; when $\beta\to 0$, there is a sharp drop in the specific characteristics related to the significant increase in the temperature in the reaction region.

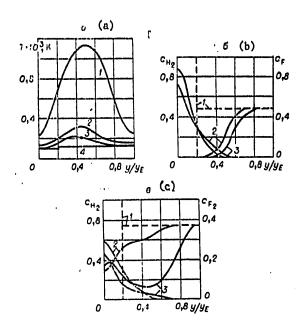


Figure 4. The profiles of the gas dynamic parameters at various values of the longitudinal coordinate; T_k = 1,100° K.

a) x is equal to 7.8 cm (1), 6 cm (2), 4 cm (3) and 0 (4);
b,c) x is equal to zero (1), 6 cm (2) and 7.8 cm (3).

A comparison was also made within the framework of the model considered here with the results of paper [11], in which the small signal gain mode is studied on the basis of complete Navier-Stokes equations. In the case where a small amount of dilutant is present in the flow, the divergence with respect to all parameters did not exceed 50%, and with a large amount of dilutant, the divergence was smaller (up to 20%). Considering the fact that the reaction rate constants and the matrix elements of the dipole moment used in [11] were not given, such a divergence must be considered satisfactory. We will note that the basic reason for the difference in the results apparently consists in the presence of a transverse pressure gradient, which is related to the considerable heat liberation in the regions where the exothermal reactions occur (it is not taken into account in our work). In this regard, one can anticipate that in the vibrational mode, where part of the energy is split out in the form of radiation, the divergence from the precise solution will decrease.

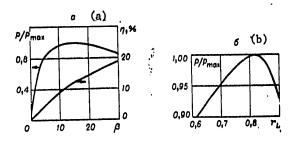


Figure 5. The laser parameters as a function of the degree of dilution (a) and the reflection factor of the semitransparent reflector (b).

In conclusion, we shall formulate the main results of this paper.

- 1. Expressions were derived for the integral characteristics of a CW chemical HF laser as a function of the governing parameters. These results make it possible to give recommendations for the optimization of laser operational modes.
- 2. Expressions for the efficiency as a function of the temperature in the precombustion chamber were compared with data derived on the basis of a quasi-one-dimensional model [8]. Despite the qualitative agreement of the nature of these functions, the two-dimensional model predicts less relative gain when making a transition to small initial levels of fluorine dissociation.
- 3. A comparison with the precise solutions of the complete system of Navier-Stokes equations [11] demonstrated that at least at large dilution levels, the model employed yields sufficiently good results.

The authors consider it their pleasant duty to express their gratitude to professor Yu.V. Lapin and M.Kh. Strelets for their numerous useful discussions of the results of the work.

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APPROVED FOR RELEASE: 2007/02/09: CIA-RDP82-00850R000100060051-8

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8225 CSO:8144/1260

PHYSICS

AN EXPERIMENTAL STUDY OF THE INFLUENCE OF THE MIXING CONDITIONS IN A LAVAL NOZZLE ON THE GAIN IN A SUPERSONIC FLOW

Novosibirsk FIZIKA GORENTYA I VZRYVA in Russian Vol 15 No 1, Jan-Feb 79 pp 97-102

[Article by B.G. Yefimov and L.A. Zaklyaz minskiy, Moscow, manuscript received 21 Mar 78]

[Text] A large amount of experimental research studying the influence of gas dynamic mixing conditions in flows of working and auxiliary gases on the inverted population of the working gas molecules has been recently carried out. This research has confirmed the theoretical conclusion of [1] that it is possible to obtain greater inversion when admixing carbon dioxide into the flow of the thermally excited auxiliary gas (nitrogen) expanding in a nozzle as compared to the expansion of a mixture prepared beforehand. In fact, in papers [2, 3] when carbon diozide and helium were injected into nitrogen heated up to a temperature of $T_0 \simeq 3,000^\circ$ K, a small signal gain of $k_0 \simeq 3$ m⁻¹ was achieved.

The higher efficiency in obtaining an inverted population when gas flows in a supersonic nozzle with the admixture of a cold working gas to the auxiliary gas is due to the fact that: a) the optimum value of the gain is obtained at greater auxiliary gas temperatures ($T_0 = 2,000-4,000^{\circ}$ K), i.e., with a greater reserve of oscillatory energy in it; b) the energy expenditures for preliminary heating of the CO_2 are reduced.

Maximally optimal from the viewpoint of obtaining the maximum inversion is the injection of the working gas into the supersonic flow of the auxiliary gas in a uniform manner over its cross-section. It is impossible to do this in practice though, since the arrangement of a large number of injection points into the supersonci flow leads to the appearance of shock waves, and possibly, to blocking of the flow. It is not possible at the present time to theoretically analyze the flow in a nozzle with the admixture of a cold gas because of the great complexity of the system of gas dynamic equations, which take into account turbulent mixing and the kinetics of oscillatory energy exchange, as well as because of the absence of reliable data on the turbulent mixing process under these conditions.

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Because of this, experimental studies have been made of the efficiency of various configurations for the insertion of the cold working gas in the flow of the auxiliary gas in a supersonic nozzle: 1) the mixing of supersonic flows of carbon dioxide and nitrogen traveling together in a channel with a constant cross-section following the nozzle [4, 5]; 2) the injection of carbon dioxide into the formed supersonic flow of nitrogen perpendicular to the direction of flow [6]; 3) the injection of carbon dioxide through slots in the walls of a flat nozzle in its subcritical section with subsequent expansion of the flow [3, 7]; 4) the injection of carbon dioxide in the vicinity of the critical cross-section of the nozzle through slots arranged in the plane of symmetry of the nozzle [2, 8].

Experiments in which the carbon dioxide was introduced through tubes with holes, where the tubes were inserted at the critical cross-section of the nozzle, were performed to obtain uniform mixture of the working gas and the auxiliary gas at the nozzle outlet [9]. However, the question of the choice of the point of injection of the working gas, and its nature to obtain a homogeneously intermixed flow at the output from the nozzle, and the opimum value of the gain, was nonetheless not sufficiently resolved in these experiments. The system of tubes, positioned in the critical cross-section of the nozzle [9], apparently provides for rather good intermixing of the gas components, but is difficult to realize in practice at small values of the height of h_\star of the critical nozzle cross-section ($h_\star \simeq 0.5$ mm) and for the case of a large mass rate of flow of the gas, when instead of one nozzle, an entire assembly is used: an array of nozzles.

Moreover, in all of the experimental works indicated here, nitrogen or air was used as the auxiliary gas, which was heated by an electric arc or in a shock wave, while the carbon dioxide gas was introduced in a mixture with helium. Since the most accessible method of heating a large quantity of auxiliary gas is the combustion of some kind of fuel (for example, CO + H₂, kerosene, benzene) in air, then it is expedient to study the admixture of the working gas (pure carbon dioxide) to the auxiliary gas, which is close in terms of its composition to the combustion products of the fuel, i.e., which contains a certain amount of carbon dioxide and water.

The purpose of the experiments set forth below is to study the influence of the location and nature of the introduction of the carbon dioxide gas and the composition of the auxiliary gas on the gain. The experiments were performed using an array, consisting of 14 flat nozzles with h* = 1.2 mm and an overall cross-sectional area of the gas flow at the output of 30 x 300 mm². The supersonic portion of the minimum length nozzles (with an inflection point) was designed to obtain a Mach number of M = 4.5 at braking parameters of p_0 = 2 · 106 Pa and T_0 = 1,400° K [10]. Air served as the auxiliary gap, in which water was added at a considerable distance from the array, while carbon dioxide was employed as the working gas.

The carbon dioxide was injected in only the subsonic portion of the nozzle. It was assumed that the admixture of ${\rm CO}_2$ in the supersonic section cannot

be effective, since turbulent mixing of two parallel supersonic flows, because of the small size of the ratio of the intensity of the turbulence to the average velocity $\left(\frac{\left(u'^2\right)^{1/2}}{u}\simeq0.01-0.02\right)$ occurs at a relatively great length

$$L = \frac{h^2 u}{4((\overline{u^2})^{1/2})} \simeq 10^2 h \quad (\text{при } l = 0,1h),$$
 (1)

where h is the nozzle height at the outlet, while l is the length of the mixing path. The introduction of streams with a large amount of motion at an angle to the supersonic flow of the auxiliary gas though leads to the appearance of intense shock waves.

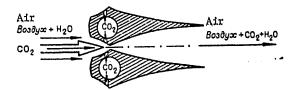


Figure 1. The configuration for the combined injection of CO₂ into the auxiliary gas flow.

In the general case, turbulent intermixing of the stream of the working gas with the auxiliary gas is realized so that the interpenetration of the large turbulent moles occurs at the outset with their subsequent "breaking up" into smaller ones. Since the transfer of the vibrational energy from the auxiliary gas to the working gas occurs only during collisions at the molecular level, this transfer will basically occur when there is turbulent mixing down to moles of a minimum size, which will already be intermixed by means of molecular diffusion.

The least path length which the particles of the working gas will travel from the point of their injection before mixing at the level of minimum sized moles can be roughly estimated from formula (1), if it is assumed that h/2 = h, and breakaway zones are formed in the region of working gas introduction, and then $\mathcal{I} \simeq h_{\star}$, and $(u^{*2})^{1/2} \simeq u$ [11]. In this case, $L_{\min} \simeq h_{\star}$, and then the greatest length will be on the order of $L_{\max} \simeq 10^{2} h_{\star}$.

It follows from these qualitative considerations and rough estimates that if the system for injecting the working gas is installed in the subsonic section of the nozzle at a distance of (0--10) h_{\star} from the critical cross-section, upstream of it, then the mixing from the minimum sized moles to the molecular level with the transfer of vibrational energy from the auxiliary gas to the molecules of the working gas will practically occur early in the supersonic flow. This circumstance governed the selection of the system for

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admixing the CO_2 , the configuration of which is depicted in Figure 1. The working gas was fed through holes in the walls of the nozzles, placed at a distance of $\simeq 3$ mm from the critical cross-section, as well as through slots arranged along the central lines of the nozzles over their entire height. The device with the slots could be moved along the flow at a distance of from 1 to $\simeq 50$ mm from the critical section.

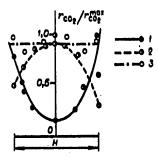


Figure 2. The distribution of the relative concentration r_{CO2}/r_{CO2}^{max} over the height H of the flow at the outlet from the nozzle.

The distribution of the carbon dioxide concentration in the supersonic flow at the outlet from the array of nozzles was monitored indirectly: based on the flow braking temperature drop, produced by the injection of cold CO2 into the heated flow of air. The braking temperature was measured using shielded Chromel-Alumel thermocouples. The CO2 concentration was estimated on the basis of the measured temperatures from the heat balance equation, with the assumption that the distribution of the concentrations and the temperatures are similar. The distribution of the CO2 concentrations at the outlet from the nozzle over its height which were obtained in this fashion and referenced to their maximum values, is shown in Figure 2, where one is for the injection of cold carbon dioxide through

holes in the walls of the nozzle; in Figure 2, where 2 is for the injection through slots positioned in the plane of symmetry of the nozzle at a spacing of = 2.5 mm from the critical section; and also in Figure 2, where 3 is for the case of combined CO2 injection, i.e., through the holes in the walls of the nozzle (60% carbon dioxide) and through the slots simultaneously. It can be seen that the injection of carbon dioxide solely through the holes in the nozzle walls or solely through central slots does not allow for a uniform distribution of its concentration over the cross-section of the flow at the outlet from the nozzle.

The small signal gain was measured from the increase in the beam intensity of a diagnostic $\rm CO_2$ laser when its passed through the supersonic gas flow at a distance of $^{\rm m}$ 10 mm from the output edges of the nozzle array. A "Svod" type photo resistor served as the receiver of the radiation.

The results of measuring the gain for various configurations of carbon dioxide injection are shown in Figure 3. All of the data were obtained at the same values of the pressure, temperature and mixture compostion. It is apparent that the greatest value of k_{ν} is achieved for the case of combination injection of the CO₂ (Figure 3, 3), in accordance with the most uni-

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uniform distribution of the CO₂ concentration at the nozzle outlet (see Figure 2). The optimal point for admixing the CO₂ is located at a distance of 2-5 mm from the critical section in the subsonic section of the nozzle. When the admixing point is removed more than 5--6 mm from the critical section, the gain initially starts to fall off sharply, and then slowly and when removed by \geq 40 mm, it approaches the value for a working gas mixture prepared beforehand (in the case of CO₂ injection only through the slots located in the plane of symmetry of the nozzle). When admixing carbon dioxide at points falling at a distance of l < 2 mm from the critical section and upstream of it, the gain likewise falls off, since the CO₂ apparently does not have time to intermix sufficiently well with the air by the time of exit from the nozzle, something which is attested to by the slight increase in the gain in the working section downstream of the output edges of the array of nozzles.

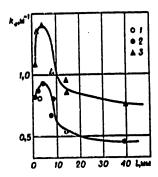


Figure 3. The influence of the position of the point of CO_2 injection relative to the critical cross-section of the nozzle on the size of the gain k_V

Key: 1. Holes in the walls of the nozzles;2. Slots in the planes of symmetry of the nozzles;

3. The combined injection of CO2.

Values of the gain are shown in Figure 4 as a function of the air braking temperature in the precombustion chamber of the setup. It can be seen that the injection of cold carbon dioxide leads to a substantial increase in the efficiency of freezing the vibrational energy in the nozzle array, and is greater the higher the temperature of the auxiliary gas.

Experiments were also performed to study the influence of the water vapor content in the auxiliary gas (the air) on the gain. Values of k_{V} are shown in Figure 5 as a function of the molar content of water vapors in the gas for the various methods of introducing the cold carbon dioxide. Curves 1 and 2 in Figure 5 were obtained when carbon dioxide was introduced through holes in the walls in the walls of the nozzles, and in this case, curve I corresponds to the intermixing of carbon dioxide at the start of the critical section 1 mm wide, while curve 2 corresponds to intermixing at a distance of 3 mm from the critical section. Curve 3 was obtained for the case of the combination injection of CO2, where in conjunction with injection through the holes in the nozzle walls, carbon dioxide was also fed in through slots arranged in the planes of symmetry of the nozzles at a distance of 2 mm from the critical section. The somewhat different nature of the behavior of the curves with the small water vapor content in the mixture, which is related to the displacement of the point of CO2 injection in an upstream direction can be clearly seen.

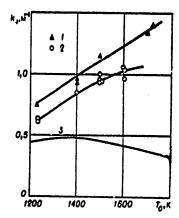


Figure 4. The gain as a function of the air braking temperature.

Key: 1. Experimental data for the combined injection of CO₂;

- Experimental data for the injection of CO₂ through holes in the walls of the nozzle;
- Calculation for the flow of a mixture of air + CO₂ + H₂O prepared beforehand, p₀ = 10⁶ Pa, r_{H2}O = 0.01.

If the carbon dioxide is introduced close to the critical section, then the (100) CO₂ level practically does not have time to populate, and the maximum value of the gain is obtained where water is absent in the mixture. When carbon dioxide is introduced at a distance of $l \ge 3$ mm from the critical section, the maximum of the gain is obtained when the water content is $r_{\rm H2O}$ = 0.01. With large amounts of water vapor, the dependence of k, on the vapor content in the working gas is similar to that for a mixture prepared beforehand. Since during the interaction of the working gas with the electromagnetic field in the resonator, to depopulate the lower (100) CO2 level, the gas should contain a certain amount of water, so that in the case where carbon dioxide is admixed in the nozzle array, its optimal content will also be equal to 0.01--0.03.

An example of the gain as a function of the amount of carbon dioxide introduced in the nozzle array is shown in Figure 6. It can be seen that the optimal value of the

relative mass rate of flow of carbon dioxide is somewhat higher than for the case of a preliminarily prepared mixture of gases, and is equal to 0.2--0.25.

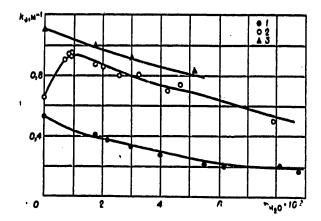


Figure 5. The influence of the water vapor content in the mixture on the gain; p_0 = 10⁵ Pa, T_0 = 1,500° K and r_{CO_2} = 0.10--0.12.

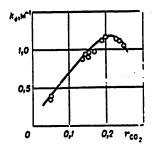


Figure 6. The gain as a function of the carbon dioxide content in the mixture; $p_0 = 10^6$ Pa, $T_0 = 1,500^{\circ}$ K and $T_{H_2O} = 0.01$.

The authors would like to thank G.V. Gembarzhevskiy and V.N. Skirda for assisting in the experiment.

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8225 CSO:8144/1260

PHYSICS

AN EXPERIMENTAL STUDY OF THE DISSOCIATION OF IODINE AND BROMINE MOLECULES IN MIXTURES OF $\mathbf{1_{2}}$ -He and $\mathbf{Br_{2}}$ -He at high temperatures

Novosibirsk FIZIKA GORENIYA I VZRYVA in Russian Vol 15 No 1, Jan-Feb 79 pp 119-121

[Article by N.A. Generalov, V.D. Kosynkin, V.A. Maksimenko and V.Ya. Ovechkin, Moscow, manuscript received 7 Sep 77]

[Text] The existing experimental data on the dissociation of molecular gases were primarily obtained under conditions where the dissociation and oscillatory relaxation processes occur separately [1]. At temperatures which are many times greater than the characteristic oscillatory temperature, the processes of oscillatory relaxation and dissociation begin to overlap. The specific features of this phenomenon were theoretically predicted in [2-8], however, only recently have the first experimental studies appeared [9-11]. This has become possible due to the simultaneous measurement of a number of parameters of a reacting system [9].

The results of studying the dissociation process of iodine and bromine molecules in a temperature range of 1,000—4,000° K, where overlapping of the dissociation and oscillatory relaxation processes is observed, are presented in this communication. The studies were made using the experimental setup of [12], which consists of a shock tube, and systems for recording the absorptivity of the gases in the visible region of the spectrum at two wavelengths as well as soft X-ray radiation.

The dissociation kinetics were studied in mixtures of I_2 and Br_2 vapors with inert gases. The profiles of the main parameters of the gas $(T_k, T_n [T_p])$ are the oscillatory and progressive temperatures; p, p, α are the pressure, density and degree of dissociation). The procedure for obtaining the indicated parameters is set forth in [9]. It has been shown that when $T_p \ge 2,000^{\circ}$ K, T_p and T_k differ markedly from each other for a considerable time (α 10 -- 20 µsec).

The results of an experimental measurement of T_k/T_p as a function of D/kT_p (D is the dissociation energy) are shown in Figure 1 for shock waves of

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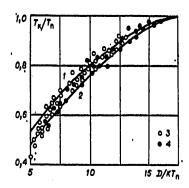


Figure 1. Values of the ratio T_k/T_p as a function of D/kT_p .

Key: 1. $\beta = 1$;

2. $\beta = 0.8$;

3. I₂;

4. Br2.

various intensities. The calculated values obtained from theory [5 - 8] are plotted in Figure 1 (1, 2) (β is a parameter defining the separation boundary of the regions of relatively fast and slow quanta exchange, where this boundary is due to the anharmonic nature of the molecular oscillations). It can be seen that the experimental and theoretical values are in agreement with each other. The absence of equilibrium with respect to the oscillatory degrees of freedom has a substantial influence on the dissociation process. The dissociation rate constant K_D becomes dependent not only on T_p but also on $T_{k^{\bullet}}$. An analytical expression for K_D/K_D^0 as a function of T_p and T_k is given in [2 - 8]:

 $\frac{H}{K_D} \frac{T_H}{T_H} = \frac{T_n}{T_H} \exp\left[\frac{D}{k} \left(\frac{1}{T_n} - \frac{1}{T_H}\right)\right], \quad (1)$

where K_D^0 is the equilibrium value of the dissociation rate constant; k is Boltzmann's constant. The value of the nonequilibrium dissociation rate constant was determined in mixtures of 20% (I_2 , Br_2) and 80% (HeNe). In the initial stage of the dissociation process, one can assume the following decomposition scheme:

$$M_2 + A \rightarrow M + M + A$$

(M_2 and M are the halogen molecules and atoms; A are the inert gas atoms), which is described by the phenomenological equation for the dissociation kinetics:

$$\frac{dn_{M_0}}{dt} = -K_{DM_0 - A}n_{M_0}n_A, \tag{2}$$

where n_{M_2} and n_A are the concentrations.

Values of ${\rm K_D}$ I₂-He in a temperature range of 2,000-4,000° K and ${\rm K_D}$ Br₂-Ne in a range of 1,000-2,300° K were determined by means of equation (2). These results are shown in Figure 2. The curves are the result of the

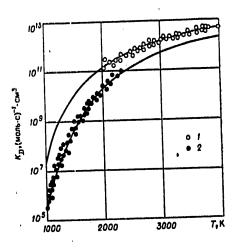


Figure 2. Values of the dissociation rate constant for iodine and bromine molecules as a function of the gas temperture.

Key: 1. I₂-He; 2. Br₂-Ne;

 K_D , (moles · sec)-1 · cm³.

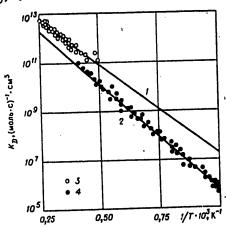


Figure 3. lnK_D^0 as a function of l/T_p .

Key: 1,2. Approximations based on Arrhenius' formula;

3. I₂-He; 4. Br₂-Ne.

 K_D (moles • sec)⁻¹ • cm^3 .

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theoretical calculation [7] based on the solution of Fokker-Planck's equation, taking into account the mutual influences of the oscillatory relaxation and dissociation processes for the hard sphere model. The good agreement of the experimental and theoretical values of $K_{\rm D}$ throughout the entire temperature range considered here should be cited.

The equilibrium values of K_D^0 were computed from formula (1). If the results obtained are presented in the form of $1nK_D^0$ as a function of $1/T_D$, then the activation energies of the I_2 and Br_2 molecules can be estimated from the slope. In fact, it can be seen from Figure 3 that this function is linear, something which attests to the correctness of Arrhenius' formula:

$$K_D^0 = Ae^{-\frac{E}{hT}}$$

where A is a constant; E is the activation energy. The value of E estimated in this fashion for iodine molecules is equal to 35.5 Kcal/mole, and \simeq 44 Kcal/mole for the bromine molecule (the dissociation energy is 45.5 Kcal/mole).

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APPROVED FOR RELEASE: 2007/02/09: CIA-RDP82-00850R000100060051-8

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8225 CSO:8144/1260

PHYSICS

THE VIBRATIONAL BAND TEMPERATURE OF CARBON DIOXIDE GAS IN A CO $_2$ + N $_2$ + H $_2$ GAS DYNAMIC LASER

Novosibirsk FIZIKA GORENIYA I VZRYVA in Russian Vol 15 No 1, Jan-Feb 79 pp 122-125

[Article by N.N. Kudryavtsev, S.S. Novikov and I.B. Svetlichnyy, Moscow, manuscript received 1 Dec 77]

[Text] The possibility of using molecular hydrogen in a CO₂ GDL [gas dynamic laser] was demonstrated in [1, 2]. The results of measuring the gain at a wavelength of λ = 10.6 µm and the intensity of the spontaneous IR radiation in the 4.3 µm band of the CO₂ molecule for the case of supersonic expansion of a mixture of CO₂ + N₂ + H₂ and at p₀ = 5--25 atm and P₀ = 800--3,000° K ahead of the nozzle are given in [3]. The vibrational temperature of the T₃ asymmetrical mode of carbon dioxide gas was determined in [4] on the basis of measurements of the radiation intensity in the 4.3 µm band with the assumption that the combined CO₂ mode (symmetrical and deformational modes) were in equilibrium with the progressive degrees of freedom (T₂ = T).

As was shown in [5], the simultaneous measurement of the spontaneous radiation intensity of $\rm CO_2$ in the 4.3 µm band, I, and the gain in the radiation of a probing $\rm CO_2$ laser, $\rm K_0$, allows for an experimental determination of the population, and consequently, the vibrational temperatures of both working lasing transition levels (001-100) of the $\rm CO_2$ molecule. Determinations of the vibrational temperatures of the asymmetrical (T₃) and combined (T₂) modes of carbon dioxide gas based on the values of the quantities $\rm K_0$ and I, measured in [3] for the case of GDL's operating on a mixture of $\rm CO_2 + \rm N_2 + \rm H_2$, are given in this paper.

The following reaction occurs in the mixture of carbon dioxide with molecular hydrogen at high temperatures:

$$CO_2 + H_2 \Rightarrow CO + H_2O. \tag{1}$$

The CO molecules and especially the H2O molecules, formed in reaction (1) can have a substantial influence on the vibrational energy exchange in

the mixtures being studied. It is also necessary to take into account the reduction in the ${\rm CO}_2$ concentration as a result of the reaction.

The calculation of the chemical composition of the mixture in the volume ahead of the nozzle was based on the experimental data of [6] for the kinetics of the overall reaction (1). According to [6], the water vapor content in the mixture is determined by the relationship:

$$\xi_{\rm H,0} = \xi_{\rm H,0}^{\rm p} \left[1 - \exp\left[-k_1 \left(\xi_{\rm H_1}^{\rm 0} \right)^{0.3} \left[M \right] t^2 \right] \right], \tag{2}$$

 $k_1=10^{10\pm0.2}\exp\left(-\frac{81.4\pm2.3}{RT}\right) \ \, (\text{cm}^3/\text{mole} \cdot \text{sec}); \ \, \xi_{\text{H}_2\text{O}}=\text{H}_2\text{O}/[\text{M}] \ \, \text{is the relative concentration of the water molecules; } \, \xi_{\text{H}_2\text{O}}^{\text{H}} \, \, \text{is the corresponding equilibrium value; } \, \xi_{\text{H}_2}^{\text{H}} \, \, \text{is the initial relative hydrogen concentration; } \, [\text{M}] \, \, \text{is the total particle density; and to is time.}$

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Hon		pa, atm	1750	1875	2000	2125	2250	2373	2500	2750	3000
3	0,1CO ₂ +0,89N ₂ + +0,0111 ₂	6.0±1,5	0,002	0,009	0,03	0,1	0,25	0,53	0.81	0,98	0,99
4	0,1CO ₂ + 0.85N ₂ + +0,05H ₂	6.0±1.5	0,01	0,07	0,2	0,72	1,8	3,2	4,2	4,4	4,5
5	0,1CO ₁ +0.8N ₂ + +0.1H ₂	6,0 + 1,5	0,03	0.13	0,47	1,4	3,1	5,6	7,0	7,2	7,3 7,3
6 7	То же	7,5-13 13+25	0,05	0.2ნ 0,51	0.9	2,5 4,1	4.7 6,0	6,8 6,8	7,1 7,1	7,2 7,2	7,3
8	0,1CO ₂ :-0.7N ₂ + -0.2H ₂	6,0±1,5	0,05	0,2	0,7	2,1	4,7	7,6	8,8	8,9	9,0

Key: A. Number of the mixture;

B. Mixture composition.

Note: The percentage water vapor content in the studied mixtures was determined for the case of t = 0.15--0.25 msec.

The amplification and radiation characteristics of the mixtures studied in [3] were measured in a time range of 0.15--0.25 msec following reflection from the end face of the tube of the incident shock wave. For this reason, the results of calculating the water vapor concentration are given in the table for this period of time in the studied mixtures as a function of the temperature and pressure in the volume ahead of the nozzle. The numeration of the mixtures in the table corresponds to the designations of the experimental curves in Figures 1-4 and in [3]. The results obtained for the 0.1 $\rm CO_2 + 0.4~N + 0.5~He~mixture$ (the quantity $\rm p_0$ corresponds to the shock

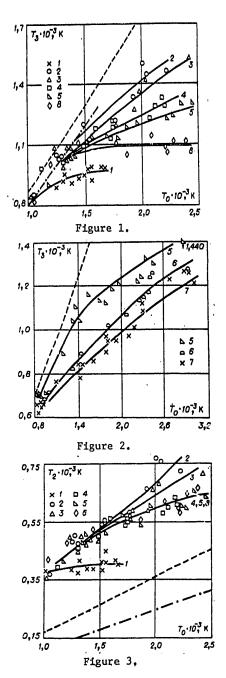
adiabat with an initial value of the prssure of 0.2 atm) and for the 0.1 $CO_2 + 0.9 N_2$ mixture ($p_0 = 6.0 \pm 1.5$ atm) are designated in Figures 1-4 and in [3] with the numbers 1 and 2 respectively. According to [7], the influence of the water molecules on the kinetics of the formation of inverted populations in a $CO_2 + N_2$ mixture must considered when the H_2O content in the mixture exceeds 0.005. It can be seen from the table at which values of T_0 the H_2O content exceeds this value.

In accordance with the table data, a specific composition of the mixture was employed in calculating the vibrational temperatures T_3 and T_2 from the measured values of K_0 and $\ I$. The presence of carbon monoxide in the mixture, which is formed in reaction (1) when using a wideband dispersion filter in the channel for recording the IR radiation, leads to the necessity of taking into account the radiation of the CO molecules in the 4.7 μm band [4].

The results of measuring the vibrational temperature of the asymmetrical CO_2 mode as a function of the temperature ahead of the nozzle for mixtures 1-5 and 8 are shown in Figure 1. T_3 for the 0.1 CO_2 + 0.8 N_2 + 0.1 H_2 mixture is shown as a function of temperature in Figure 3 for various pressures. The temperature in the critical nozzle section, T_{\star} , is shown in Figures 1 and 2 with the dashed lines, and with the dashed and dotted line for mixture 1.

A comparison of vibrational temperature values, obtained in this work, with the values of T_3 obtained for the same mixtures in [4], shows that determining T_3 using the approximate method of [4] leads to values overstated by $40\text{--}120^\circ$ K in a temperature range ahead of the nozzle of $800\text{--}2,500^\circ$ K. It was shown in [4] that because of the assumption of the thermalization of the combined mode, the approximate method permits the obtaining an upper estimate of T_3 . It follows from a comparison of Figures 1 and 2 with the results of [4] that the approximate method correctly reflects the basic laws governing the change in T_3 as a function of T_0 , T_0 , and the composition of the mixtures. The following belong to these governing laws: an increase in T_3 and in the difference T_4 and T_3 with an increase in T_3 with an increase in the initial hydrogen concentration and an increase in the pressure from 5 to 25 atm. The greatest values of T_3 are achieved with the expansion of the binary mixture T_4 and T_5 bound be noted that the values T_8 for mixture 1 is substantially lower than the value T_8 for mixtures T_8 for mixture 1 is substantially lower than the value T_8 for mixtures T_8 .

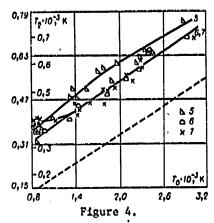
The vibrational temperature of the combined CO_2 mode as a function of the temperature ahead of the nozzle for mixtures 1-5 and 8 at p_0 = 6.0 \pm 1.5 atm and for the mixture 0.1 CO_2 + 0.8 N_2 + 0.1 H_2 when the pressure varies from 5 to 25 atm are shown in Figures 3 and 4. The dashed lines in Figures 3 and 4 show the gas temperature in the working cross-section of the flow



for mixtures 2-8, while the dashed and dotted line is for mixture 1. For all of the mixtures studied under the conditions of this work ($T_0 = 800-3,000^{\circ} K$, P_0 = 5--25 atm), a rising curve for T_2 as a function of T_0 is observed. We will note the high degree of nonequilibrium of the combined CO2 mode: the vibrational temperature exceeds the gas temperature by 1.5-2.0 times. For mixtures 4, 5 and 8 with an additional hydrogen content of 0.05, 0.1 and 0.2 $(\phi_0 = 6.0 \pm 1.5 \text{ atm})$, the values of T_2 throughout the entire range of T_0 = = 800--2,500° K are in agreement within the limits of the measurement precision. For mixture 3 ($\xi_{\rm H2}^0$ = 0.01), elevated values of T_2 are observed at $T_0 \ge 1,600^{\circ}$ K. In this same range of temperatures of To, binary mixture 2 possesses the greatest vibrational temperature T_2 . The value of T_2 for mixture 1, which contains helium, is substantially lower than for mixtures 2-5, and 8 with added amounts of hydrogen,

The influence of the pressure on the vibrational temperature of the combination CO_2 mode for a mixture with $\xi_{H2}^0 = 0.1$ is illustrated by curves 5-7 in Figure 4. The measured values of T_2 or $p_0 = 7$ —25 atm practically coincide (see Figure 4, 6, 7) throughout the entire investigated range of $T_0 = 800$ —3,000° K. When $p_0 = 6.0 \pm 1.5$ atm (see Figure 4, 5), the magnitude of T_2 is 60—100° K higher than for pressures of 7.5—25 atm.

Thus, the increase determined in [3] for the gain and in the relative inverted population of the $\rm CO_2$ lasing levels when molecular hydrogen is added to a binary mixture of $\rm CO_2$ + $\rm N_2$ in the amount of 1--5% is due to the more significant



reduction in the population of the lower lasing level as compared to the upper one (see curves 2-4 in Figures 1 and 3). The reduction in the gain (see curves 5 and 8 in Figures 3 and 4 (3)) at high hydrogen concentrations (0.1--0.2) is determined predominantly by the reduction in the population of the upper lasing level T3 (see curves 5 and 8 in Figures 1 and 3). With an increase in the gas pressure in the volume ahead of the nozzle, the reduction in the gain noted in the mixture of 0.1 CO2 + + 0.8 N₂ + 0.1 H₂ is related to the more rapid relaxation of the asym-

metrical CO₂ mode as compared to the combination mode (see curves 5-7 in Figures 2-4).

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