

# OPTIMIZATION OF THERMAL REGIME OF CONTINUOUS CO<sub>2</sub>-LASERS WITH DIFFUSION COOLING\*

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*Mathematical methods for optimizing parameters of the CO<sub>2</sub>-laser, realized using numerical computer simulation, are proposed. The results of numerical calculations coincide with the results of the experimental data, at a partial discrepancy, the reasons associated with the non-optimal consideration of the proposed recombination model on the wall of the O-tube in the reaction  $O + O^W \rightarrow O_2$  were established. The results of the work can be fully used to optimize various designs of continuous CO<sub>2</sub>-lasers.*

**KEY WORDS:** *laser, temperature, recombination, atom, gas, concentration, current density*

## 1. INTRODUCTION

From all the types of lasers for industrial applications, electrically excited CO<sub>2</sub>-lasers are in a great demand [1-4]. Nowadays, not only new designs and models of CO<sub>2</sub>-lasers with different output parameters are being created, but also a significant number of research is being performed on optimization of the laser characteristics, i.e., the studies on determining the conditions when limiting values of power, best stability, beam divergence, mode structure, pulse shape, spectral purity, etc. are achieved. The optimization of laser characteristics is a combination of fundamental mathematical solutions and numerical methods aimed to find and identify the best parameter options from a variety of alternatives that permit one to avoid the complete enumeration and estimation of the possible ones [5-8].

It should be noted that the improving the energy characteristics [9] is one of current central problems.

## 2. MATHEMATICAL MODEL OF THE DYNAMICS OF THE CHEMICAL COMPOSITION OF THE GAS MIXTURE OF CO<sub>2</sub>-LASER

The method of dynamics calculation the of chemical composition is based on the difference of two time scales: slow ( $\sim 10^2$  s), associated with irreversible changes in the

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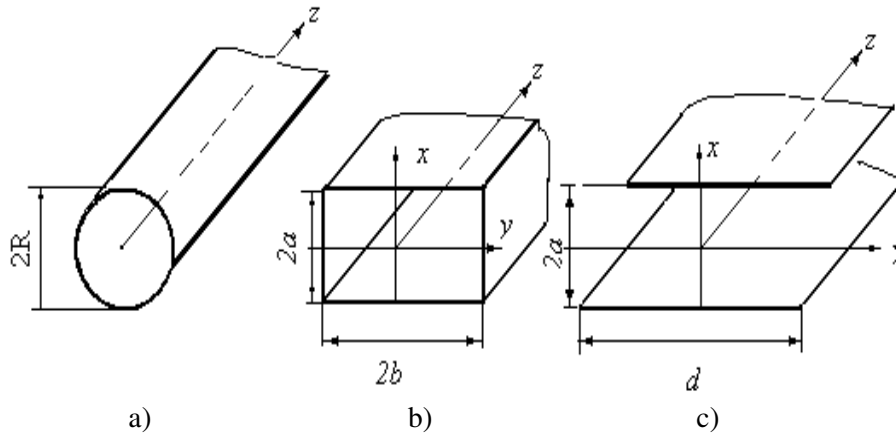
chemical composition in an additional volume, and rapid ( $\sim 10^{-2}$  s) which has relation with the dissociation processes, recombination, and diffusion of particles. To describe the changes in the chemical composition, stationary diffusion equations are used which follow from the balance equations and motion of particles of type  $\alpha$  in the diffusion mode:

$$\nabla \cdot D_\alpha \nabla n_\alpha + I_\alpha = 0, \quad (1)$$

where  $D_\alpha$  and  $n_\alpha$  are the diffusion coefficient and the concentration of  $\alpha$ -components;  $I_\alpha$  is the source density of the particles of this class, formed and dying as a result of chemical reactions. Equation (1) should be complemented by the boundary conditions reflecting the formation and death of particles on the walls of the discharge channel:

$$\vec{e} D_\alpha \nabla n_\alpha = S_\alpha, \quad (2)$$

where  $S_\alpha$  is the surface density of the particle sources of the class  $\alpha$  and  $\vec{e}$  is a unit normal to the surface. The solution of the system of Eq. (1) with boundary conditions (2) depends on the geometry of the discharge chamber. The considering discharged structures with size indication and the coordinate systems used for studding are shown in Fig. 1.



**FIG. 1:** The discharge cameras: cylindrical (a), rectangular in a cross section (b), slit (c)

For cases presented in Figs. 1(a) and 1(b), by averaging Eq. (1) over the cross section taking into account the boundary conditions (2) and omitting the averaging symbol for simplicity, we obtain:

$$D_\alpha \frac{\partial^2 n_\alpha}{\partial z^2} + \gamma S_\alpha + I_\alpha = 0, \quad (3)$$

$$N_\alpha = V_\alpha (\gamma S_\alpha + I_\alpha), \quad (7)$$

The change in the components concentration in the additional volume  $V$  is described by the set of balance equations:

$$V \frac{dn_\alpha^0}{dt} = N_\alpha + L_\alpha, \quad (8)$$

where  $L_\alpha$  is the particles source of class  $\alpha$  due to the chemical reactions on the surface of the stabilizer of the gas composition of the mixture and other structural elements.

### 3. MATHEMATICAL MODEL OF OPTIMIZATION OF GAS-DISCHARGE CO<sub>2</sub>-LASER

For this case, the velocity constants for the formation of nitrogen oxides are small and their concentrations are insignificant [6,7]. Therefore, nitrogen oxides in the dissociation kinetics are not taken into account. The reactions describing the dissociation kinetics of CO<sub>2</sub> in the high-frequency (HF) discharge are similar to the reactions occurring in the plasma of a direct current glow discharge [2].

The dynamics of changes in concentrations of  $n_\alpha^0$  in the additional volume is determined by the system of balance equations:

$$V \frac{dn_1^0}{dt} = S_c \beta J_{3c} - SD_1 \frac{\gamma}{2} (n_1 - n_1^0), \quad (9)$$

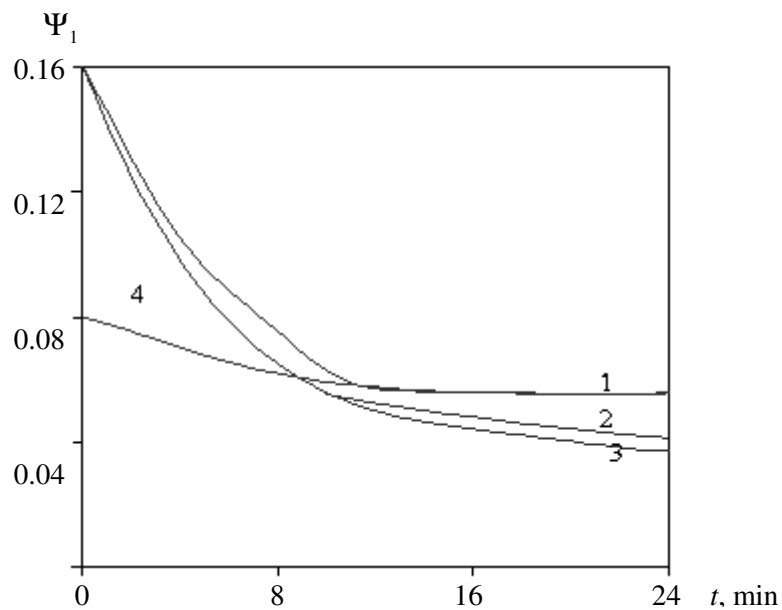
$$V \frac{dn_2^0}{dt} = SD_2 \frac{\gamma}{2} (n_2 - n_2^0) + Q_3 (n_4^0)^2 n_1^0, \quad (10)$$

$$n_1^0 - n_3^0 = n^0, \quad (11)$$

$$V \frac{dn_4^0}{dt} = SD_3 \frac{\gamma}{2} (n_3 - n_3^0) - 2V \frac{dn_2^0}{dt} - \nu, \quad (12)$$

where  $L_1 = S_c \beta J_{3c}$  is the source of CO<sub>2</sub> on the surface of the gas composition stabilizer with the active area  $S_c$ ;  $\beta$  is the parameter determining the reducing properties of the stabilizer ( $0 \leq \beta \leq 1$ );  $\nu$  is the velocity of oxygen loss due to the implementation, adsorption and chemical absorption on the electrodes and other structural elements;  $n_1^0$  is the concentration of CO<sub>2</sub> molecules during filling;  $J_{3c}$  is the flux density of CO molecules on the stabilizer;  $Q_i$  are the constants of chemical reactions, where  $i$  is the reaction number. The value  $J_{3c}$  is determined by the ratio

The results of the simulation of the stationary values of  $\text{CO}_2$ ,  $\text{O}_2$ ,  $\text{CO}$ , and  $\text{O}$  concentrations, as well as the degree of dissociation of  $\text{CO}_2$  molecules from various factors when a discharge is excited by a direct current in a cylindrical capillary in comparison with experimental data [7] are presented in Figs. 3 and 4. When calculating the dynamics of the chemical composition of plasma,  $\alpha = 0$  was taken as zero approximation, and  $\alpha = 0.5$  was used when calculating the stationary values of the concentration which provide the fast convergence of the computational process. The constants  $Q_i$  are obtained similarly to [2], and the dissociation cross section by an electron impact of  $\text{CO}_2$  and  $\text{O}_2$  molecules is gotten from [9].

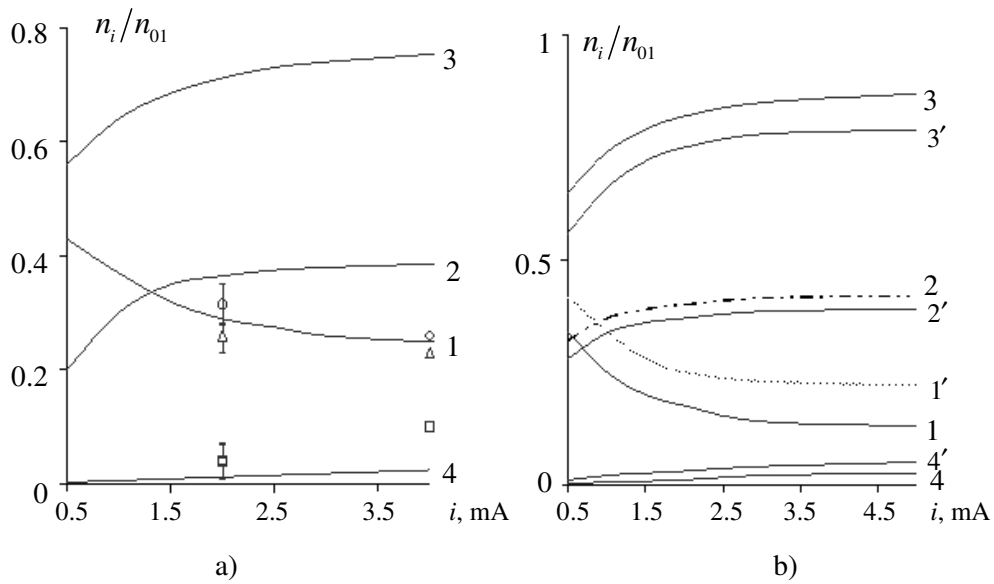


**FIG. 2:** The change in time of the mole fraction of  $\text{CO}_2$ ,  $\Psi_1$  in the additional volume (1-3) and the capillary (4), when  $v = 0$  (1, 4),  $10^{-3}$  (2),  $10^{-2}$  (3)

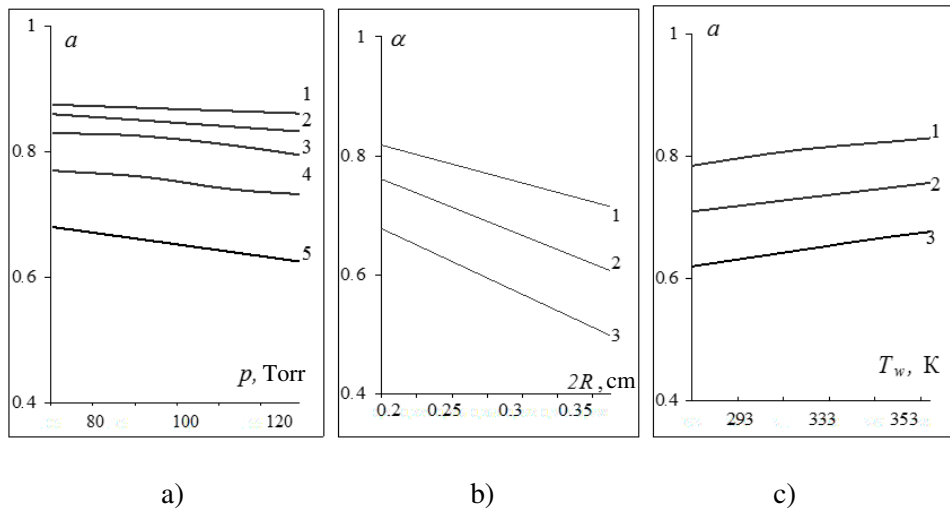
For the constants  $Q_1$ , the results of [1] obtained for molybdenum glass were used. Taking into account the difference in materials,  $Q_1$  was adjusted downward by 20–30% in simulations, that improved the matching between the calculated and experimental data. For HF discharge the approximation,

$$Q_1 = 10^{-17} (0.46 + 25 / j) \text{cm}^4 \text{s}^{-1} \quad (16)$$

was used, where  $j$  is the effective value of the conduction current density.



**FIG. 3:** The dependence of the relative concentration of  $n_i/n_1^0$  particles on the discharge current in the steady-state mode, CO<sub>2</sub> - 1, O<sub>2</sub> - 2 CO - 3, O - 4: (a)  $p = 100$  Torr,  $R = 0.125$  cm,  $T_w = 293$  K for the mixture of CO<sub>2</sub> : N<sub>2</sub> : He : Xe = 1:1:8:0,  $\Delta$  - O<sub>2</sub>,  $\square$  - O,  $\circ$  - CO<sub>2</sub> are experimental data [7]; (b)  $p = 100$  Torr,  $R = 0.1$  cm,  $T_w = 293$  K for 1:1:4:0.2 (1-4), for a mixture 1: 1: 8: 0 (1'-4')



**FIG. 4:** The dependence of the degree  $\alpha$  on: pressure (a) 1:1:4:0.2, when  $I = 0.5$  mA (1), 3 (2), 2 (3), 1 (4), 0.5 (5); the capillary diameter  $2R$  (b) for the mixture of 1:1:8: 0, when  $I = 0.5$  mA (1), 2(2) 1 (3); from the temperature of the external surface of the capillary  $T_w$  (c), when  $R = 0.125$  cm for the mixture of 1:1:8:0,  $I = 0.5$  mA (1), 2(2), 1(3)

## 5. OPTIMIZATION OF THE THERMAL REGIME OF THE CO<sub>2</sub>-LASER

When calculating the average gas temperature in the discharge, the stationary heat conduction equation was used by reason of the period of field oscillations is much less than the temperature relaxation time with HF excitation:

$$\nabla \cdot \lambda \nabla T + u = 0, \quad (17)$$

where  $\lambda(\vec{r})$ ,  $u(\vec{r})$ ,  $T(\vec{r})$  are the coefficient of thermal conductivity and the volume density of the power of heat sources and the temperature of the gas, respectively. The heat equation was solved for circular, rectangular in cross section and slit discharge chambers. The equality of the temperature on the wall to  $T_w$  was used as a boundary condition.

For the coefficient of thermal conductivity of the mixture of gases, we have [11]:

$$\lambda = \sum_{\alpha} \lambda_{\alpha} \left[ 1 + \Psi_{\alpha}^{-1} \sum_{\beta} A_{\alpha\beta} \Psi_{\beta} \right]^{-1} = \sum_{\alpha} \lambda_{\alpha} \beta_{\alpha}, \quad (18)$$

where  $A_{\alpha\beta}$  are values that weakly depend on temperature;  $\lambda_{\alpha}$  is the thermal conductivity of the  $\alpha$ -component of the mixture, whose dependence on temperature follows a linear law in a wide temperature range:

$$\lambda_{\alpha} = \lambda_{0\alpha} \left[ 1 + \kappa_{\alpha} (T - T_0) \right], \quad (19)$$

where  $\lambda_{0\alpha}$  is a thermal conductivity at temperature  $T_0$ ;  $\kappa_{\alpha}$  is a constant for given gas. Using Eq. (19), for the coefficient of thermal conductivity of the mixture (2.24), we obtain the linear relationship:

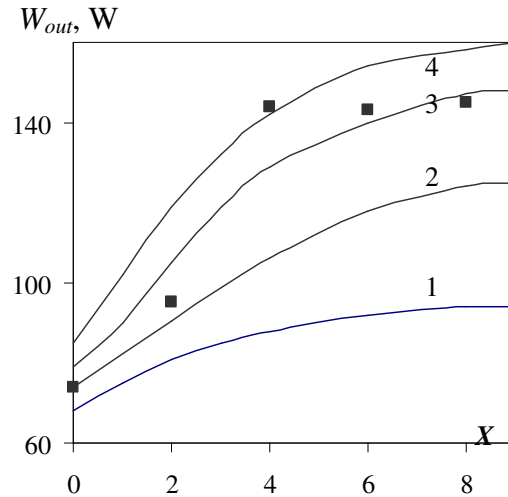
$$\lambda = \lambda_0 + \lambda_1 T, \quad (20)$$

where  $\lambda_0 = \sum_{\alpha} \beta_{\alpha} \lambda_{\alpha 0} (1 - \kappa_{\alpha} T_0)$  and  $\lambda_1 = \sum_{\alpha} \beta_{\alpha} \lambda_{\alpha} \kappa_{\alpha}$  are the coefficients determined by the composition of the mixture.

The solution of Eq. (17) using Eq. (20) for thermal conductivity permit one to obtain the temperature distributions and the average temperatures for discharges in chambers of various configurations. Taking into account that the distribution of heat sources  $u(\vec{r})$  is determined by the spatial distribution of electrons and using for the last one the results in [2] in the case of HF excitation as well as the data of [12] for direct-flow discharges in a cylindrical capillary, it can be shown that the maximum temperature difference between the plasma and the wall in a wide range of the discharge conditions together with the average gas temperature  $\langle T \rangle$  are determined by the expressions [13]:

$$W = 1.71ad\bar{I}_s(X - 1.25), \quad (24)$$

where  $X$  is a gain excess over loss;  $\bar{I}_s$  is an average cross-section saturation intensity. The numerical coefficients in Eq. (24) describe the difference in the distribution of the radiation field from the field of a plane wave. When calculating  $X$  and  $\bar{I}_s$ , data of [14] were used.



**FIG. 5:** The dependence of  $W_{out}$  for a  $\text{CO}_2$ -laser on the percentage of CO,  $X = (\psi_{03}/15.3)100\%$  when  $k = 1(1), 3(2), 7.5(3), 9(4)$ ; — is simulation results and ■ — is experimental data [14]

The composition of the mixture in the steady state was calculated according to the method described with the difference that  $\psi_{03}$ , the non-zero mole fraction of CO when filling, was used as an additional parameter. The effect of the gold coating of the electrodes was taken into account by multiplying the coefficient  $k$  of recombination velocity constant of the CO and O molecules on the wall  $Q_1$ . The best fitting of the calculated and experimental data corresponds to the value of  $k = 7.5$ . Estimated time  $\tau$  for establishing the equilibrium concentrations of the components worse fits the experiment data. Thus, according to the calculations, when  $k$  changes from 1 to 7.5,  $\tau$  decreases from 30 to 4.5 min, while as stated in [12],  $\tau$  decreases from 35 to 1 min. The possible reason for this difference is associated with mistaking into account the recombination on the wall of O atoms in the reaction  $O + O^W \rightarrow O_2$ .

## 6. CONCLUSIONS

The mathematical methods for the parameters optimization of a  $\text{CO}_2$ -laser are proposed and implemented with numerical simulation. The computation results

coincide with the results of experimental data; with partial mismatching, the reasons have been found that relate to nonoptimal accounting of the proposed recombination model on the tube wall of O atoms in the reaction of  $O + O^W \rightarrow O_2$ . The obtained results could be applied for the optimization of various designs of continuous CO<sub>2</sub>-lasers.

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