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Numerical modelling of kinetic processes in the plasma of a supersonic electric-discharge CO laser excited by a microwave discharge

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***Abstract*.** **A model is developed for calculating pump parameters of the active medium of a supersonic electric-discharge CO laser excited by a microwave discharge. A variant of the design of such a radiation source is described. Calculations are performed both for the 'hot' variant of the radiation source, when the gas mixture is produced by burning the fuel in a gas generator, and the 'cold' variant, when the gas mixture is supplied to the discharge region from gas vessels. The regions of optimal values of the reduced field strength and parameters of the gas mixture for the 'cold' variant are determined. It is shown that the parameters of the active medium obtained in the 'hot' variant correspond to the parameters of highly efficient radiation sources reported in the literature.**

Keywords: *CO laser, microwave discharge, radiation source based on the combustion products of the hydrocarbon fuel.*

1. Introduction

CO lasers feature a high efficiency (up to 63 %) and have a high output power. These lasers emit at shorter wavelengths (4.8 – 8.2 μm) than CO_2 lasers, which is important for some applications. Electric-discharge CO lasers with the supersonic flow of the working mixture, in which the active medium is excited in the discharge region and the supersonic flow is used for cooling the gas mixture and removing waste products, are the most promising for the development of high-power and highly efficient radiation sources. Such lasers combine the high output power inherent in gas-dynamic lasers with the high efficiency of electric-discharge lasers [1]. The development of supersonic-flow electric-discharge lasers operating on the combustion products of the hydrocarbon fuel was reported in [2]. It was pointed out that, having the advantages of radiation sources with the open cycle (not so high requirements to the cooling and circulation systems as in lasers with the closed cycle; the absence of the contamination of the active medium by the products of plasma-chemical reactions and the deterioration of the optical parameters of the medium during operation), the service life of such lasers is longer than that of conventional supersonic electric-discharge CO lasers due to the production of the gas mixture during lasing. Other advantages of these lasers are the possibility to increase the specific energy input and to establish the optimal (for excitation of oscillations) reduced field strength without the use of an electron gun by employing the associative ionisation during the supersonic expansion of a gas mixture. The requirements to the purity of the gas mixture, which are very strict in other lasers, are substantially milder if the hierarchy of times [3]

$$\tau_{VV} < \tau_{eV} \leqslant \tau_{dis} < \tau_{VT} \leqslant \tau_{d} \leqslant \tau_{ch}$$

is fulfilled, where τ_{dis} is the residence time of the mixture in the discharge region; τ_{eV}, τ_{d}, and τ_{ch} are the characteristic times of excitation of vibrational levels by a direct electron impact, dissociation, and in chemical reactions, respectively; and τ_{VV}, τ_{VT} are the characteristic times of the vibrational and translational relaxation, respectively.

The active medium of electric-discharge CO lasers is usually pumped by a dc or high-frequency discharge. Excitation of the active medium by a microwave discharge offers certain advantages over excitation by discharges in other frequency ranges. These advantages are the absence of electrodes in the microwave discharge, the absence of the pump power losses on ballast resistances and in near-electrode layers, and the closeness of the pump field frequency to the frequency of elastic collisions of plasma electrons with neutral particles [4, 5]. In addition, a microwave discharge is more stable than discharges in other frequency ranges, and its application can provide an increase in the specific energy input without the development of the discharge contraction. A microwave frequency of 2.45 GHz used, as a rule, for pumping electric-discharge CO lasers in industrial applications is of interest because the corresponding pump radiation wavelength is comparable with the plasma column length.

In this paper we studied a supersonic electric-discharge CO laser in which the active medium was excited by a microwave discharge in a grooved waveguide (Fig. 1). Such a waveguide can be treated as a rectangular waveguide with a longitudinal slit in the middle of a wide wall. This slit is non-emitting for the fundamental H_{10} mode because it does not intersect the lines of the surface current. Screening plates are jointed to the edges of the slit. The length of plates in the direction perpendicular to the longitudinal axis was chosen

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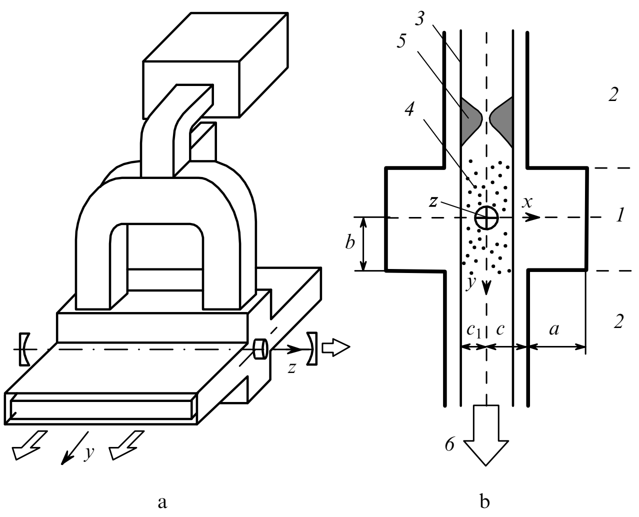

Figure 1. Schematic view of the design of a microwave-pumped supersonic gas-discharge CO laser (a) and the cross section of the grooved waveguide (b): (*1*, *2*) groove and slit regions; (*3*) flight channel; (*4*) discharge region; (*5*) supersonic nozzle; (*6*) gas flow direction; a, b, c, and c_1 are the groove depth and half-width, half-width of slits, and half-width of the gas-discharge channel, respectively.

so that the radiation power decay at their end was 40–60 dB. The cross section of the grooved waveguide is shown in Fig. 1b. The figure presents the coordinate system, the characteristic dimensions of this waveguide structure and the position of flight-path channel (*3*), and shows groove region (*1*) and two slit regions (*2*).

The main advantage of the grooved waveguide in this construction is that this waveguide structure is open and is naturally conjugated with the gas flow. The gas mixture can be supplied to the discharge region from vessels ('cold' variant) or can be produced by burning a fuel in a gas generator ('hot' variant), which provides a considerable mass rate of gas flow. The mixture is cooled due to adiabatic expansion during its outflow through a supersonic nozzle.

2. Formulation of the problem and description of the calculation algorithm

Kinetic processes in the discharge under study were numerically simulated, first, to find the region of admissible values of parameters of excitation and the gas flow for the 'cold' variant of a supersonic gas-discharge CO laser and, second, to calculate the parameters of the active medium created in a flow produced by burning a fuel in a gas generator. The one-dimensional problem was considered and plasma parameters were assumed constant in planes perpendicular to the gas flow. The boundary effects were neglected.

The groove area along the flow was divided into twenty segments; the field strength and plasma parameters were assumed constant within each of them. In this case, the relative change in the field strength distributed according to the cosine law does not exceed 10 %. It was assumed that microwave radiation in the grooved waveguide propagates in the fundamental H_{11} mode. The field strength was determined for each of the segments. The electron energy distribution function (EEDF) f was found by solving numerically the Boltzmann equation in the form

$$\varepsilon^{1/2}\frac{\mathrm{d}f}{\mathrm{d}t}=\frac{2}{3}\frac{e^{3/2}}{m_{\mathrm{e}}}E^2\frac{\partial}{\partial\varepsilon}\left(\varepsilon^{3/2}\frac{\nu_{\mathrm{m}}}{\nu_{\mathrm{m}}2+\omega^2}\frac{\partial f}{\partial\varepsilon}\right)+\frac{2m_{\mathrm{e}}}{e^{1/2}}\frac{\partial}{\partial\varepsilon}\left(\tilde{\nu}_{\mathrm{m}}\varepsilon^{3/2}f\right)$$

$$+\frac{2M_{\mathrm{e}}kT}{e^{1/2}}\frac{\partial}{\partial\varepsilon}\left(\tilde{\nu}_{\mathrm{m}}\varepsilon^{3/2}\frac{\partial f}{\partial\varepsilon}\right)+\sum_{t,j}\left[N^{(t)}f(\varepsilon+\varepsilon_j)Q_j^{(t)}(\varepsilon+\varepsilon_j)\right.$$

$$\left.\times(\varepsilon+\varepsilon_j)-N^{(t)}f(\varepsilon)Q_j^{(t)}(\varepsilon)\varepsilon\right]\left(\frac{2}{em_{\mathrm{e}}}\right)^{1/2}=0. \qquad (1)$$

Here, e, m_{e}, and ε are the electron charge, mass, and energy, respectively; E and ω the electric field strength and frequency, respectively; $\nu_{\mathrm{m}}(\varepsilon)=\sum_t\nu_{\mathrm{m}}^{(t)}(\varepsilon)$; $\nu_{\mathrm{m}}^{(t)}(\varepsilon)$ is the transport frequency of collisions of electrons with neutral particles of the tth component of the gas mixture; $N^{(t)}$ is the concentration of particles of the tth component; $Q_j^{(t)}$ is the cross section of the jth inelastic process involving particles of the tth component; ε_j is the decrease in the electron energy in the jth inelastic scattering process; $\tilde{\nu}_{\mathrm{m}}=\sum_t\nu_{\mathrm{m}}^{(t)}/M^{(t)}$; $M^{(t)}$ is the mass of particles of the tth component. Eqn (1) was solved according to [6] by the method of finite differences by using the inverse substitution. Superelastic collisions were neglected. The cross sections of elastic (in calculations of ν_{m}) and inelastic electron–molecular collisions presented in [7] were used. The average energy W_E imparted to an electron from the pump field per unit time, the rate constants $X_j^{(t)}$ of excitation of vibrational levels of CO and nitrogen by a direct electron impact, the average energy W_{p} imparted by electrons to vibrations of CO and nitrogen molecules per unit time, and the ionisation and attachment frequencies ν_{i} and ν_{at} were calculated from the found EEDF by using the relations

$$W_E=\sum_{\varepsilon=0}^{100\ \mathrm{eV}}\varepsilon\Delta\varepsilon\left[\frac{2}{3}\frac{e^{3/2}}{m}E^2\frac{\partial}{\partial\varepsilon}\left(\varepsilon^{3/2}\frac{\nu_{\mathrm{m}}}{\nu_{\mathrm{m}}^2+\omega^2}\right)\frac{\partial f}{\partial\varepsilon}\right],$$

$$X_j^{(t)}=\left(\frac{2}{m_{\mathrm{e}}}\right)^{1/2}\sum_{\varepsilon=0}^{100\ \mathrm{eV}}Q_j^{(t)}(\varepsilon)\varepsilon f(\varepsilon)\Delta\varepsilon\,,$$

$$W_{\mathrm{p}}=\sum_{t,j}h\nu_j^{(t)}N^{(t)}X_j^{(t)},$$

$$\nu_{\mathrm{i,at}}=\left(\frac{2}{m_{\mathrm{e}}}\right)^{1/2}\sum_t\sum_{\varepsilon=0}^{100\ \mathrm{eV}}N^{(t)}Q_{\mathrm{i,at}}^{(t)}(\varepsilon)\varepsilon f(\varepsilon)\Delta\varepsilon\,.$$

Here, $N^{(t)}$ ($t=1,\ 2$) is the concentration of CO and nitrogen molecules; $h\nu_j^{(t)}$ is the energy of the jth vibrational state of molecules of the tth component of the gas mixture; $\Delta\varepsilon$ is the electron energy interval within which the EEDF value is assumed constant. The electron concentration was determined from its balance equation, which was written separately for a self-sustained discharge maintained by the pump field ('cold' variant) and in the case of a high electron concentration at the input to an electric-discharge section caused by associative preionisation and typical for a supersonic electric-discharge CO laser operating on combustion products ('hot' variant).

The balance equation for the electron concentration n_{e} for the 'cold' variant has the form

$$u\frac{\mathrm{d}n_{\mathrm{e}}}{\mathrm{d}y}=(\nu_{\mathrm{i}}-\nu_{\mathrm{at}})n_{\mathrm{e}}-\gamma n_{\mathrm{e}}^2. \qquad (2)$$

Here, u is the gas flow velocity; y is the spatial coordinate along the flow; and γ is the three-body recombination coefficient. The empirical dependence $\gamma = 8.25 \times 10^{-8}(E/N)^{-0.851}$ obtained in [8] was used, where γ is expressed in $cm^3\ s^{-1}$, E/N is expressed in 10^{-16} V cm^2, and N is the concentration of neutral particles.

The solution of Eqn (2), taking into account the boundary condition $n_e(y = -b) = n_0^c$, is the electron concentration in the 'cold' variant

$$n_e = \frac{v_i - v_{at}}{\gamma + \tilde{\gamma}\exp[-(v_i - v_{at})(y - b)/u]}, \quad \tilde{\gamma} = \frac{v_i - v_{at}}{n_0^c} - \gamma, \quad (3)$$

where b is the half-width of the groove. The electron concentration n_0^c at the input to the electric-discharge section was set equal to $10^2\ cm^{-3}$.

The parameters of the active medium created in the flow produced by burning the fuel in the gas generator were calculated by using the specified pressure, composition and velocity of the gas flow in the gas-discharge channel. The electron concentration n_0^h in the gas flow at the input to the electric-discharge section was set equal to $10^{11}\ cm^{-3}$. This value was obtained experimentally [9] in the study of associative dissociation in nitrogen during its adiabatic supersonic expansion. The initial electron concentration n_0^h relaxes during the propagation of the flow in the electric-discharge section to the value determined by the reduced field strength. Therefore, the electron concentration n_e in each cross section of the flow can be written in the form

$$n_e = n_0^h + \delta n(y), \quad (4)$$

where $\delta n(y)$ is the correction to the initial value caused by the action of the pump field and gas-kinetic processes. The balance equation for the electron concentration has the form

$$\frac{d(n_0^h + \delta n)}{dt} = (v_i - v_{at})(n_0^h + \delta n) - \gamma(n_0^h + \delta n)^2. \quad (5)$$

By solving Eqn (5), we found the expression for the electron concentration in the 'hot' variant

$$n_e = n_0^h + \frac{B}{A}\{\exp[A(y - b)] - 1\},$$

$$A = \frac{v_i - v_{at} - 2n_0^h\gamma}{u}, \quad B = \frac{n_0^h}{u}(v_i - v_{at} - n_0^h\gamma). \quad (6)$$

The calculation was performed for each spatial step along the y axis, and the calculated parameters were determined by spatial averaging.

3. Results of numerical modelling

We calculated the 'cold' variant by studying parameters characterising the pump efficiency as functions of the composition, pressure, and velocity of the gas flow, as well as of the reduced field strength. The following parameters were calculated: the specific volume energy input $P_e = W_E n_e$; the quantity $\tilde{e} = P_e\tau/P_{CO}$ (where $\tau = 2b/u$ is the time of flight through the discharge region) corresponding to the specific energy input per unit pressure (1 Torr) of CO for the time of flight through the discharge region; the energy $W_{CO} = P_e\tau/N_{CO}$ per one CO molecule for the time of flight through the discharge region; the specific mass energy input $W_m = P_e\tau/m_V$ (where $m_V = m_0\sum_{t=1}^{K} m_t N^{(t)}$ is the mass of the gas unit volume, m_0 is the atomic mass unit, m_t and $N^{(t)}$ is the relative molecular mass and concentration of particles of the tth component of the gas mixture, and K is the number of components); and the pump efficiency $\eta = W_p/W_E$. We studied the $CO - N_2 - Ar - He$ mixture. Boltzmann equation (1) and balance equation for the electron concentration (2) were solved numerically for a set of initial data, and the characteristic excitation time $\tau_p = (X_1^{(1)}n_e)^{-1}$ of the first vibrational level of CO was determined. Then, the velocity u of the gas mixture flow was selected by the method of gradient descent so that τ_p differed from the gas residence time in the discharge region by no more than 1 %. For the power of a microwave generator $P_g = 10$ kW, assuming that the active medium is pumped homogeneously, the length of the discharge region along the optical resonator axis $L_d = P_g/(4bc_1P_e)$ was calculated (where $c_1 = 1$ cm is the half-width of the gas-discharge channel). The results of calculations for the 'cold' variant are presented in Figs 2 – 5.

The parameters $\tilde{e}$, P_e, W_{CO}, and W_m increase with increasing the reduced field strength (Fig. 2) because the electron concentration and energy W_E imparted to electrons from the pump field per unit time increase. For a fixed pump power, the increase in the reduced field due to the increase in the specific volume energy input leads to a decrease in the discharge-region length, which can occur only to a certain limit because, on the one hand, the gain per pass in the resonator decreases, and on the other hand, the matching of

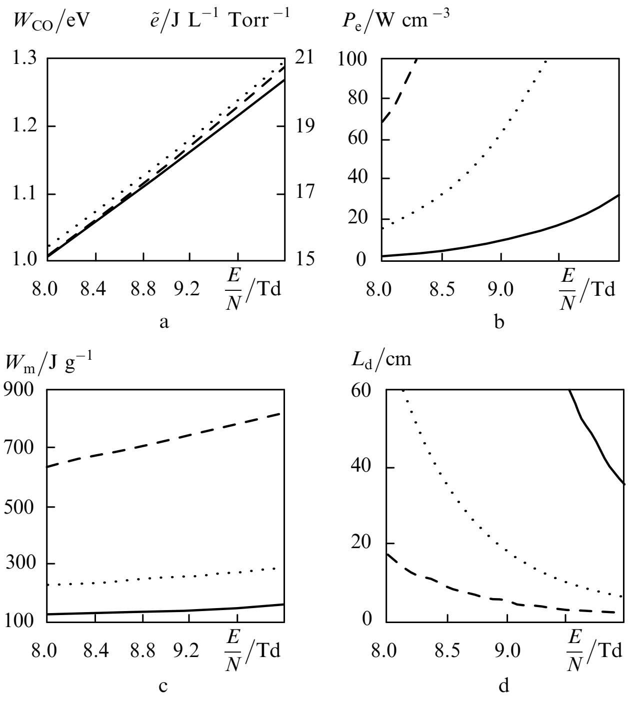

Figure 2. Dependences of the parameters $\tilde{e}$ and W_{CO} (a), P_e (b), W_m (c), and L_d (d) on the reduced field for the 'cold' variant. The $CO:N_2:Ar = 5:10:85$ mixture, $p = 10$ Torr (solid curves), the $CO:N_2:He = 5:10:85$ mixture, $p = 20$ Torr (dashed curves), and the $CO:N_2:Ar:He = 5:10:40:45$ mixture, $p = 15$ Torr (dotted curves).

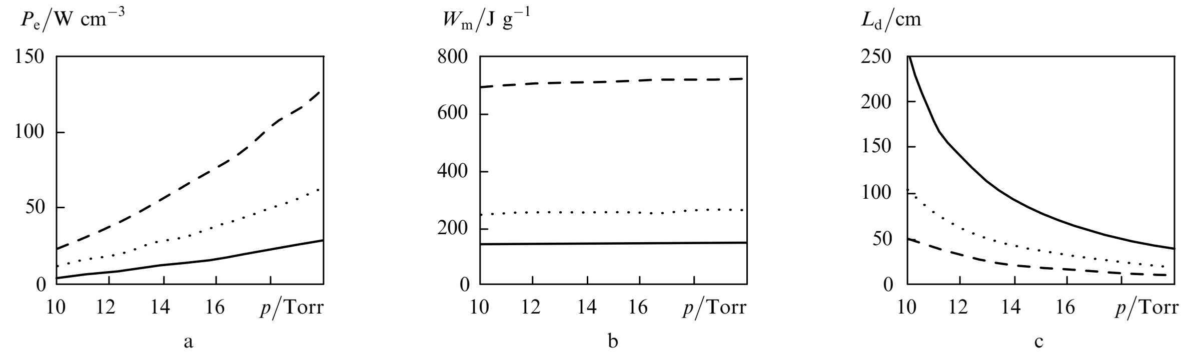

Figure 3. Dependences of the parameters P_e (a), W_m (b), and L_d (c) on the gas mixture pressure p for mixtures $CO:N_2:Ar = 5:10:85$ (solid curves), $CO:N_2:He = 5:10:85$ (dashed curves), and $CO:N_2:Ar:He = 5:10:40:45$ (dotted curves) for $E/N = 8.5$ Td.

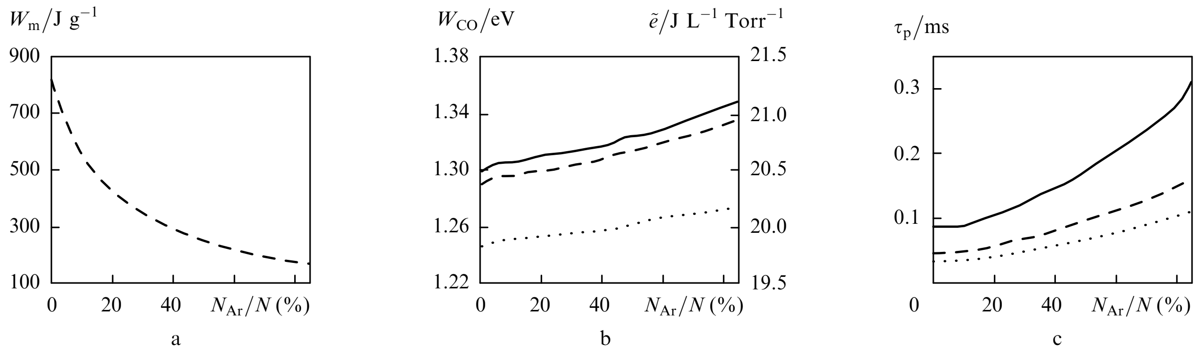

Figure 4. Dependences of the parameters W_m (a), W_{CO} and $\tilde{e}$ (b), τ_p (c) on the percentage of Ar in the 5 % CO : 10 % N_2 : Ar : He mixture for $E/N = 10$ Td, $p = 10$ (solid curves), 20 (dashed curves), and 30 Torr (dotted curves).

the load in the form of a plasma column with elements of the waveguide path becomes worse. The mater is that, because the electric-discharge section is a microwave resonator, its length should be no less than half the radiation wavelength in the waveguide and should be equal to a few halves the wavelength to provide good matching. In addition, as the reduced field increases, a part of the electron energy W_p spent to excite vibrations of CO and N_2 molecules decreases. For this reason, the optimal value of the reduced field for mixtures under study lies between 8.5 and 9.5 Td and shifts to large values of E/N for 'heavy' mixtures (containing considerable amounts of argon).

The increase of the parameter P_e with increasing the pressure of the gas mixture (Fig. 3) is explained by the increase in W_E. The specific mass energy input is almost independent on the pressure because the increase in W_E is compensated by the increase in the gas-mixture density. As the pressure of the gas mixture increases, the concentration of emitting particles increases but the length L_d of the discharge region decreases. Therefore, the optimal pressure 12 – 18 Torr exists at which the required amplification is provided per round trip in the resonator. For mixtures enriched with argon, these values can be higher since L_d in these mixtures is larger (see Fig. 3c), which is explained by a lower energy W_E because argon atoms have no low-lying energy levels with a high excitation cross section.

As the percentage of argon in the mixture is increased compared to the content of helium, the energy input W_m decreases (Fig. 4), which is natural because in this case the specific weight of the mixture increases. The parameters $\tilde{e}$

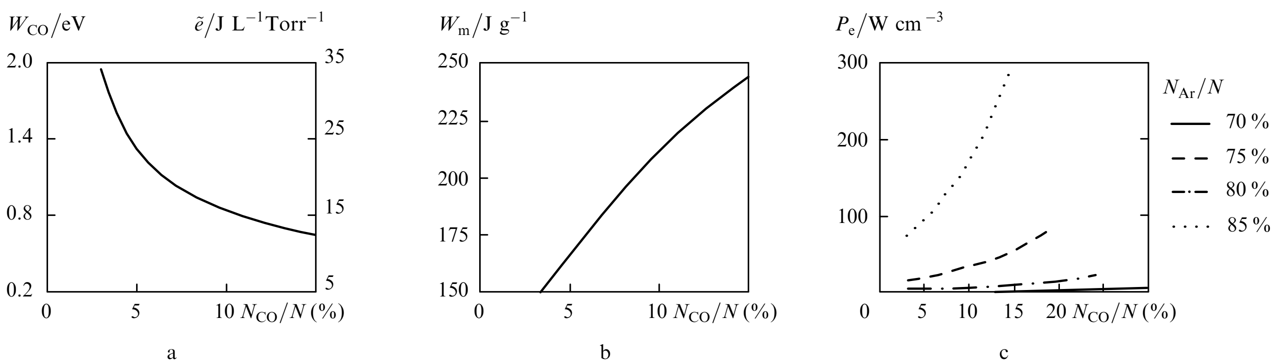

Figure 5. Dependences of the parameters $\tilde{e}$ and W_{CO} ($N_{Ar}/N = 85$ %) (a), W_m ($N_{Ar}/N = 85$ %) (b) and P_e (c) on the percentage of CO in the $CO:N_2:Ar$ mixture for $E/N = 10$ Td and $p = 15$ Torr.

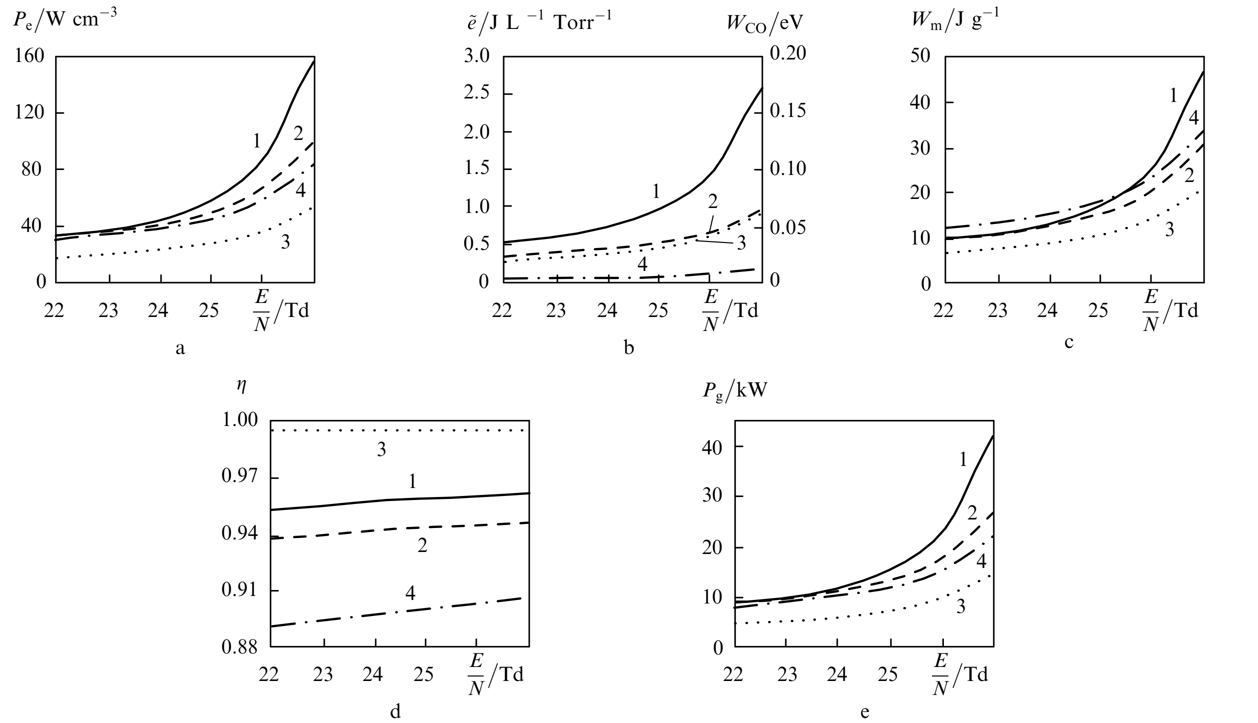

Figure 6. Dependences of the parameters P_e (a), $\tilde{e}$ and W_{CO} (b), W_m (c), η (d), and P_g (e) on the reduced field E/N for four compositions of the gas mixture (Table 1) produced by burning the hydrocarbon fuel in the gas generator.

and W_{CO} increase insignificantly because the required time of flight of the mixture through the discharge region increases. The latter circumstance is explained by the decrease in the excitation rate $X_1^{(1)}$ of the first vibrational level of CO due to the increase in the electron temperature caused by a decrease in the inelastic electron losses (argon atoms have no low-lying energy levels with a high excitation cross section).

The dependences of parameters $\tilde{e}$ and W_{CO} on the percentage of CO in the mixture are presented in Fig. 5. One can see that these parameters decrease with increasing the CO concentration. The mass energy input increases because the molecular masses of CO and N_2 are identical, while the volume energy input P_e increases with increasing the CO concentration. The increase in P_e is caused by the increase in the parameter W_E because the cross section of vibrational excitation of CO molecules is higher than that of nitrogen molecules, and the increase in the electronic energy spent for excitation of vibrational levels is compensated by a greater amount of energy transferred to electrons from the pump field.

The parameters of the 'hot' variant were studied for four compositions of the gas mixture produced by burning the hydrocarbon fuel in the gas generator (Table 1). Figure 6 presents the dependences of the specific volume energy input P_e, parameters $\tilde{e}$ and W_{CO}, energy input W_m, pump efficiency η, and power P_g of the microwave generator on the reduced field E/N [P_g is the microwave power required for pumping the discharge region of size $2 \times 30 \times 4.5$ cm (the first and second numbers are the height and width of the flight channel, respectively, and the third number is the length of the discharge region along the flow)] for the calculated energy input P_e, which is assumed homogeneous.

It is known [1] that the stationary lasing regime is achieved when the parameter $\tilde{e}$ exceeds 1.7 J L^{-1} Torr^{-1}. One can see from Fig. 6b that the first mixture satisfies this requirement for the reduced field strength exceeding 26 Td. This mixture is characterised by rather large values of the parameter η. At present various domestic commercial 2.45-GHz microwave generators of the magnetron type are available which provide powers satisfying the requirements illustrated in Fig. 6d (for example, a 50-kW KIE-5 source). The energy input W_m for the 'hot' variant proved to be low (up to 48 J g^{-1}). According to [8], its threshold is 300 J g^{-1}, but probably this is valid only for the two-component CO – N_2 mixture used in [8] for which the parameter W_m is in fact the energy input per 'pumped' molecule, whereas the mixtures under study contain several components and are

Table 1. Composition and parameters of the combustion products of the hydrocarbon fuel and air.

Mixture number	Fuel	α_{gg}	p_g/kPa	T_g/K	u/m s^{-1}	Composition of the CO : N_2 : O_2 : H_2 : Ar gas mixture (%)
1	Acetylene – air	0.397	4.2	100	1140	7.9 : 71.2 : 15.4 : 3.9 : 0.9
2	Benzene – air	0.404	4.2	100	1160	13.9 : 67.2 : 11.1 : 6.9 : 0.9
3	Kerosene – air	0.37	4.2	213	1700	23.3 : 52 : 19.5 : 0.6
4	Kerosene – air	0.37	4.2	100	990	13.2 : 63.2 : 10.4 : 12.3 : 0.8

Note: α_{gg} is the oxidiser excess coefficient in a gas generator; p_g and T_g are the gas pressure and temperature in the gas-discharge channel.

better characterised by the parameter W_{CO}. In the region $E/N > 25$ Td, most of the dependences drastically grow due to the increase in the electron concentration in this region caused by the increase in the ionisation rate.

4. Conclusions

The calculation performed for the 'cold' variant shows that there exists the optimal reduced field strength caused by the decrease in the discharge-region length and in the fraction of electron energy spent for excitation of vibrations of CO and N_2 molecules with increasing the value of E/N. The optimal reduced field strength is 8.5 – 9.5 Td, and increases in 'heavy' mixtures (containing considerable amounts of argon). It follows from the figures presented in the paper that the percentage of argon in mixtures should exceed 40 %. The increase in the argon percentage is expedient because it reduces the rate of VT processes and results in the broadening of the plateau of the vibrational distribution function. The optimal content of CO in the mixture is 5 % – 15 % and depends on the argon percentage.

It follows from the results of calculations that the parameters of the active medium obtained in the 'hot' variant of the laser correspond to the parameters of highly efficient radiation sources reported in the literature. Thus, a small microwave-pumped 10-kW CO laser operating on the combustion products of the hydrocarbon fuel ballasted with air can be realised. At the same time, the 'cold' variant of the radiation source has better parameters determining the pump efficiency, which means that it is reasonable to add a correcting argon-containing gas mixture into the working mixture produced by burning the hydrocarbon fuel.

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