METHOD FOR CALCULATING GAS DISCHARGE CHAMBER CHARACTERISTICS
WITH CONSIDERATION OF THE BOUNDARY LAYER

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Calculation of gas passage through a channel with parallel walls [1] is a problem of independent interest (in particular, with regard to describing turbulence [2]). Among the numerous methods for solving such problems (see, e.g., [3]), none is universal.

Of great practical interest is the calculation of gas discharge chambers, used in plasma chemistry and lasers. In that case it is necessary to study the gas dynamic equations in combination with equations describing oscillatory excitation of the gas molecules by the glow discharge. The well-known difficulties of constructing a simple and effective method for calculation of a gas flow with consideration of the boundary layer at high Reynolds number ($\sim 10^4$-10^5) are complicated by specific problems related to oscillatory excitation.

The development of a method for numerical solution of the gas discharge chamber problem with consideration of the boundary layer is the goal of the present study.

Even under laminar boundary layer conditions, which occur most often at characteristic gas flow parameters in the gas discharge chamber (pressure ~ 10 kPa, gas flow velocity ~ 100 m/sec, h ~ 5 cm, L ~ 50 cm), the incorrectness of the one-dimensional jet approximation is obvious. Oscillatory excitation of molecules by a glow discharge in the presence of boundary layers should lead to intense heating of the gas in those layers and significant inhomogeneity in the gasdynamic parameters. Other reasons necessitating treatment of the problem in the two-dimensional approximation are heat loss from the heated gas to the chamber wall and possible heterogeneous relaxation (on construction details) of oscillatorily excited molecules.

Significant calculation difficulties arise because of the geometry of the gas discharge chamber (Fig. 1): in practical chambers the number of "calibers" $L/h \geqslant 15 \gg 1$. For numerical calculation of the boundary layer as parameter values characteristic of such chambers, the number of divisions required along the y-axis is $N_y \sim 10^2$, while along the x-axis $N_x \geqslant 10^3$, i.e., the number of points in the spatial grid may reach $\geqslant 10^5$, which of itself makes a numerical solution of the problem by traditional methods problematic. Under conditions of intense inhomogeneity, one must use a nonuniform step size, which not all of the known methods permit [3].

In the present study we will develop a method for calculating gas discharge chamber characteristics based on the summary approximation method [4]. The solution of this problem is of practical interest for clarifying the effect of gas flow structure on pumping efficiency in long gas discharge chamber channels. The most widely used gas discharge chamber system is shown in Fig. 1, where 1 is the forechamber, 2 is the actual gas discharge chamber with glow discharge, and 3 is the output chamber; the chamber walls serve simultaneously as electrodes (A, anode, C, cathode, while the arrow indicates the direction of gas flow).

We consider a gas which is a mixture of anharmonic oscillators with inert atoms (for example, N_2:He, CO:He, etc.) with CO_2 added to several percent (such mixtures are used in technological lasers). We now formulate our basic physical assumptions. Oscillatory excitation of molecules is produced by a glow discharge of specified power density $jE = W_d(x, y)$ and an oscillatory efficiency η_d; a fraction of the power $1 - \eta_d$ is expended in directly heating the gas. The heat from the heated gas arrives at the wall, the specific heat of which we is assume infinitely high .

The equations describing the steady-state boundary layer of the flow of viscous thermally conductive gas have the following form in Cartesian coordinates (ρ, p, T are the gas density, pressure, and temperature, $V = \{u, v, 0\}$ is the velocity vector):
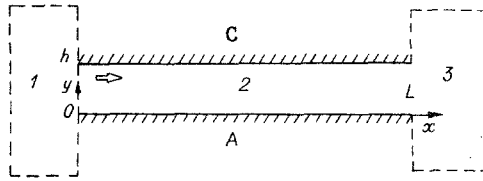

Fig. 1

the continuity equation

$$\partial u/\partial x + \partial v/\partial y + u\partial \ln \rho/\partial x + v\partial \ln \rho/\partial y = 0; \tag{1}$$

the projection of the law of conservation of momentum on the x-axis

$$\rho u\partial u/\partial x + \rho v\partial u/\partial y + dp/dx = \partial \tau/\partial y + F_x; \tag{2}$$

the law of conservation of energy

$$\rho c_p(u\partial T/\partial x + v\partial T/\partial y) - udp/dx = Q_v; \tag{3}$$

$$Q_v = \partial q/\partial y + \tau\partial u/\partial y + Q_{rel} + (1 - \eta_d)jE, \qquad Q_{rel} = \rho(E_N - E_{Ne})/\tau_N, \tag{4}$$

where the thermal source terms Q_v denote, respectivley, heat liberation due to thermal conductivity, internal friction, oscillatory energy relaxation, and direct heating of the gas by the discharge;

$$\tau = \mu\partial u/\partial y; \tag{5}$$

the dynamic viscosity coefficient

$$\mu = \mu_0(T/T_0)^{0.76}; \tag{6}$$

the thermal flux

$$q = \lambda\partial T/\partial y; \tag{7}$$

λ is the thermal conductivity coefficient ($\lambda = \mu c_d/Pr$); Pr is the Prandtl number; F_x is the volume force.

We now derive a consequence of system (1)-(3) convenient for the calculation procedure. With consideration of elementary relationships for an ideal gas, it follows from Eq. (3) that $-(u\partial \ln \rho/\partial x + v\partial \ln \rho/\partial y) = (\gamma - 1)/\gamma \cdot Q_v/p - u/\gamma \cdot d \ln p/dx$. Combining this with Eq. (1), we obtain

$$\partial u/\partial x + \partial v/\partial y = (\gamma - 1)/\gamma \cdot Q_v/p - u/\gamma p \cdot dp/dx. \tag{8}$$

We then subtract Eq. (2) from Eq. (8) and divide the result by u:

$$\partial(v/u)/\partial y = (1 - M^2)/\rho u^2 \cdot dp/dx + (\gamma - 1)/\gamma \cdot Q_v/pu - (\partial \tau/\partial y + F_x)/\rho u^2, \tag{9}$$

where the Mach number

$$M = u/\sqrt{\gamma RT}. \tag{10}$$

An important relationship follows from Eq. (9): considering that

$$\lim_{\substack{y\to 0+0 \\ y\to h-0}} (v/u) = \lim_{\substack{y\to 0+0 \\ y\to h-0}} (\partial v/\partial y)/(\partial u/\partial y) = 0, \tag{11}$$

we integrate Eq. (9) from 0 to h:

$$0 = dp/dx \int_0^h (1 - M^2)/\rho u^2 \cdot dy - \int_0^h [(\partial \tau/\partial y)/\rho u^2 - (\gamma - 1)/\gamma \cdot Q_v/pu] \, dy,$$

whence

$$dp/dx = \int_0^h [(\partial \tau/\partial y)/\rho u^2 - (\gamma - 1)/\gamma \cdot Q_v/pu] \, dy \Big| \int_0^h (1 - M^2)/\rho u^2 \cdot dy. \tag{12}$$

For the specific (per unit mass of gas) oscillatory energy E_N, we have

$$\rho u\partial E_N/\partial x + \rho v\partial E_N/\partial y = \partial J_v/\partial y - \rho(E_N - E_{Ne})/\tau_N + \eta_D jE, \tag{13}$$

where

$$J_v = \rho D^*\partial E_N/\partial y \tag{14}$$

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is the diffusion flux of oscillatory energy; E_{N_e} is the equilibrium value of E_N:

$$E_{N_e} = X_{N_2} R T_1 / (\exp(T_1/T) - 1);$$ (15)

T_1 = 3380 K is the energy of the first oscillatory level of the N_2 molecule;

$$R = 83,14 \Big/ \sum_i \mu_i X_i;$$ (16)

μ_i is the molecular weight in atomic units; X_i is the fraction of gas i in the mixture.

Thus, for the numerical solution we will use Eqs. (2), (9), (13), and

$$\rho u c_d \partial T^* / \partial x + \rho c_d \partial T^* / \partial y = \partial(q + u\tau) / \partial y + Q_{rel} + (1 - \eta_d) jE + u F_x,$$ (17)
$$T^* = T + u^2 / 2c_d,$$

as well as Eqs. (4)-(7), (10)-(16) and the boundary conditions at the input and walls of the chamber:

$$v(x, 0) = v(x, h) = 0, \ u(x, 0) = u(x, h) = 0, \ v(0, y) = 0.$$

Here u(0, y) is a specified function; T*(x, 0) = T*(x, h) = T^*_c is a specified quantity; T*(0, y) = T^*_0; p(0, y) is the pressure at the input.

We describe the numerical solution algorithm. Specifying u(x_0, y), p(x_0, y), T*(x_0, y) (at the chamber input x_0 = 0, T*(0, y) = T^*_0), a) we define dp/dx for a given x_0 from Eq. (12); b) from Eq. (9) we find v(x_0, y) (the transverse velocity component in the given section; we use Eq. (11) for the boundary conditions); c) knowing dp/dx and the transverse velocity profile, we make a step in x(x → x_0 + Δx): by solving system (2), (13), (17) with corresponding boundary conditions, we find T*(x_0 + Δx, y), E_N(x_0 + Δx, y), and u(x_0 + Δx, y).

The system (2), (13), (17) can be solved for T*, E_N, u by the summary approximation method [4], i.e., we divide the system into a series of sequentially solvable sybsystems, namely (we omit boundary conditions everywhere):

I) $dT^*/dx = 0$, $dy/dx = v/u$, $du/dx = 0$, $dy/dx = v/u$, $dE_N/dx = 0$,
$d/dx = \partial/\partial x + dy/dx \cdot \partial/\partial y$;

II) $\rho u c_d \partial T^* / \partial x = \partial(q + u\tau)/\partial y$, $\rho u \partial u/\partial x = \partial\tau/\partial y$, $\rho u \partial E_N/\partial x = \partial J_v/\partial y$,
$q = \lambda \partial T/\partial y$;

III) $\partial T^*/\partial x = 0$, $c_d \partial T/\partial x + u \partial u/\partial x = 0$, $\rho u \partial u/\partial x + dp/dx = 0$, $u \partial u/\partial x + 1/\rho \cdot dp/dx = 0$, $\rho u \partial E_N/\partial x = 0$;

IV) $\rho u c_d \partial T^*/\partial x = Q_{rel} + (1 - \eta_d) jE$, $\rho u \partial u/\partial x = 0$, $\rho u \partial E_N/\partial x = -\rho(E_N - E_{Nd})/\tau_N + \eta_d jE$.

Having determined u, E_N, T*(x_0 + Δx, y) and using steps «a», «b», the values of v, dp/dx(x_0 + Δx, y), we take the next step in x, etc. The division along the y-axis is uniform and comprises N_y = h/Δy = 50-100 intervals. The step in x is chosen from the condition of stability of the numerical integration of subproblem I-IV; the number of such nonuniform divisions along the x-axis $N_x \gtrsim 10^3$. The obvious advantage of the proposed method is the possibility of calculating gas discharge chamber characteristics over an arbitrary length, more precisely, one such that L/h ≫ 1.

The numerical solution of the system of equations was verified by calculating gas flow rate at the input, in various cross sections, and at the chamber output, together with the energy balance. Although the calculation does not employ difference analogs of the conservation laws, the mass and energy balances agree with a completely satisfactory accuracy ⩽ 3%.

Another test procedure is to calculate the steady-state distribution of gasdynamic parameters in the chamber in the absence of a glow discharge. For an arbitrary velocity profile at the gas discharge chamber input, u(0, y), as L → ∞ the calculation yields a u(L, y) at the output which approaches a Poiseuille flow.

At first glance, the use of the laminar boundary layer approximation may raise doubts, since under conditions typical of high-flow lasers, Re ∿ 10^5 or more. However careful study of the question reveals that for the gas flow parameters studied, Re < Re_{cr}, and there is no reason to doubt the validity of the approximation used.
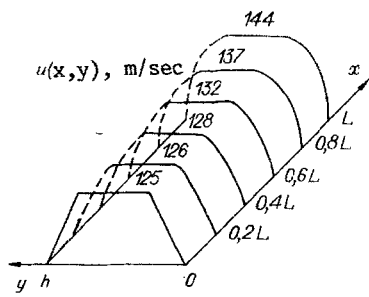
Fig. 2

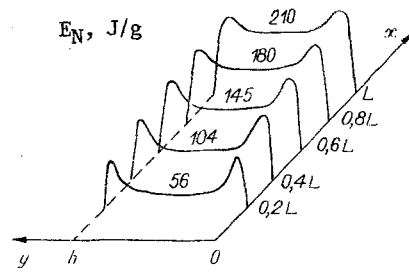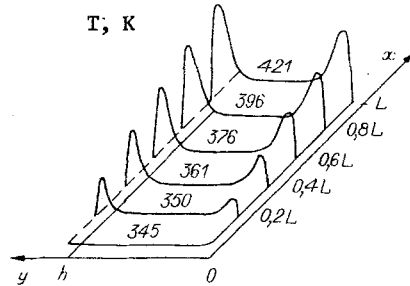Fig. 3

Fig. 4

As an example, we consider calculation of a gas discharge chamber with characteristic parameters: $L/h = 25$, specific gas flow rate 2 g/(cm²·sec), symmetrical longitudinal velocity profile at the input (Fig. 2), and mean velocity $\bar{u} = \frac{1}{h} \int_0^h u(0, y)\, dy = 100$ m/sec. We specify the volume power of the glow discharge homogeneous over the gas discharge chamber space (with the exception of the near-electrode regions), $jE = 3 \cdot 10^6$ W/m³, discharge efficiency $\eta_d = 0.95$ [5]. For a mixture $CO_2:N_2:He = 2:49:49$ we take relaxation constants such that $(p\tau_{N_2-N_2})^{-1} = 10^{-3}$ (Pa·sec)⁻¹, $(p\tau_{N_2-He})^{-1} = 5.1 \cdot 10^{-5}$ (Pa·sec)⁻¹ at 300 K.

Figure 2 shows the longitudinal component of gas flow velocity u(x, y) in various sections of the gas discharge chamber, with velocity values on the chamber axis of symmetry noted. It is evident that the velocity profile smooths toward the output, while the size of the boundary layer increases. With motion toward the gas discharge chamber output, the gas heats up and the pressure increases. The calculations also consider the presence of near-electrode regions in the discharge. jE is specified in a narrow region near the electrodes in accordance with known values of the anode and cathode potential drop, while the discharge efficiency at the cathode $\eta_d|_c = 0$. Also considered was the dependence of τ_N on $\Theta = T_N/T$, the ratio of the oscillatory to the translational temperature, where when some threshold value Θ_{cr} is reached, τ_N falls by two or more orders of magnitude [5]. Relaxation of oscillatorily excited molecules on the gas discharge chamber walls is considered by the condition at the wall

$$D_v^* \partial E_N/\partial y \big|_{\substack{y=0 \\ y=h}} = -\, 2\varepsilon_v/(2 - \varepsilon_v)\, \sqrt{\gamma RT}/4 \cdot E_N \big|_{\substack{y=0 \\ y=h}},$$

with excited molecules reaching the wall by diffusion and relaxing with an accommodation coefficient ε_v [6] (it was assumed that $\varepsilon_v = 1$).

Because of the lower flow velocity at the walls, the gas there remains in the chamber longer and is "pumped" more intensely (Fig. 3, which shows the distribution of oscillatory energy density $E_N(x, y)$ over the gas discharge chamber, gives E_N values on the chamber axis of symmetry). Figure 4 shows the temperature distribution T(x, y) over the gas discharge chamber, with temperature values on the axis noted. It is evident that the gas is heated more in the boundary layer as a result of relaxation. In the direct vicinity of the wall, the gas is colder due to heat loss to the wall. Despite the high discharge efficiency which was specified ($\eta_d = 0.95$), when the boundary layer is considered, the fraction of oscillatory energy is quite low, comprising $\leqslant 0.6$ in the total chamber energy balance.

Within the framework of the system of equations used herein, an analogous study could be performed for the presence of turbulence, it being sufficient to add turbulent transport coefficients to the equations where required.

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GENERALIZED RELAXATION EQUATIONS FOR VIBRATIONAL AND ROTATIONAL
MOLECULAR KINETICS IN GAS FLOWS

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A system of kinetic equations for the distribution functions of gas particles over quantum states (over vibrational and rotational molecular levels) is usually used to describe nonequilibrium relaxation processes in molecular gases [1]. Here we consider impurity relaxation of a molecular gas in a monatomic gas flow, when molecular collisions can be neglected and the distributions of gasdynamic parameters are known.

The kinetic equations are in this case

$$\frac{dN_i}{dt} = n_g \sum_j (K_{ij}N_j - K_{ji}N_i),$$ (1)

where N_i is the population of the i-th molecular quantum level with energy E_i, satisfying

the normalization condition $\sum_i N_i = 1$; $K_{ij}(T)$ are rate constants of molecular transi-

tions from state j into state i during collisions with atoms of the gas flow, having temperature T and density n_g and satisfying the detailed balance rule $K_{ij}N_j^* = K_{ij}N_i^*$; N_i^* are molecular equilibrium Boltzman distributions over quantum states, $N_i^* = g_i \exp(-E_i kT)/S$; g_i is the statistical weight of the state; and S is the partition function for the system of levels under consideration, $S = \sum_i g_i \exp(-E_i/kT)$.

For known dependences of K_{ij} on quantum numbers and temperature, as well as for known distributions of the gasdynamic parameters of the monatomic gas, Eqs. (1) can be solved numerically. However, the numerical solutions of the kinetic equations are not always convenient, as a large amount of calculations is required, particularly if it is necessary to take into account the large number of quantum levels.

Besides, the shape of the constants $K_{ij}(T)$ is usually unknown, and the absence of reliable constants leads to the necessity of using semiempirical dependences with adjustable parameters in solving the kinetic equations, selected by comparison with experiment. This also increases the bulk of calculations, and the problem of choosing an adequate set of rate constants, describing experimental data, remains nonsimple. The matter is that rate constants with different dependences on quantum numbers and temperature can lead to nearly equal distributions in the populations of molecular quantum levels.

Here we propose to represent the populations N_i in the form of an expansion in orthogonal functions. As a result, the system of kinetic equations (1) transforms to an equivalent system of moment equations, characterized by some set of time relaxations ω_{km}^{-1}, which in some