CALCULATION OF HIGH POWER RELATIVISTIC BEAMS WITH CONSIDERATION OF COLLISION EFFECTS

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Numerical calculation of relativistic charged particle beams moving in axisymmetric systems in which the presence of a residual neutral gas is possible is considered. In this content it is essential to consider phenomena related to collisions between charged particles and neutrals (for example, ionization and charge transfer). Algorithms are constructed for numerical modeling of ionization processes within the framework of the ERA program complex [1]. Solutions of model and practical problems are presented as examples. Such problems were studied previously in [2, 3] where ionization processes were considered by a more complex method requiring a greater volume of calculations but valid at lower pressures.

We will consider the following mathematical formulation of the problem. In a closed axisymmetric region $\bar{G} = G + \Gamma$ with boundary Γ we must calculate the motion of a beam of charged particles bearing electric charge e (for the feature we will assume that the "primary" charged particles beam consists of electrons) with rest mass m. In the region G there may exist a neutral gas under a pressure p which is a function of (r, z), the coordinates of the observation point.

The equation of motion of the electron beam particles has the form

$$\frac{d}{dt}\left(\gamma m \frac{d\mathbf{R}}{dt}\right) = e\mathbf{E} + \frac{e}{c}[\mathbf{V} \times \mathbf{H}], \tag{1}$$

where γ is the relativistic factor, c is the speed of light, t is time, $\mathbf{V} = d\mathbf{R}/dt$, $\mathbf{E}$, $\mathbf{H}$ are the electric and magnetic fields, and $\mathbf{R}$ is the radius vector of the electron.

Particle coordinates and velocities are specified at the initial moment:

$$\mathbf{R}|_{t=0} = \mathbf{R}_0, \ \mathbf{V}|_{t=0} = \mathbf{V}_0. \tag{2}$$

The electric field $\mathbf{E} = -\mathbf{grad}\,\varphi$ is found by solution of the Poisson equation for the potential

$$\Delta\varphi = -4\pi\rho \tag{3}$$

with boundary conditions

$$\varphi|_\Gamma = g, \ \ \partial\varphi/\partial\mathbf{n}|_\Gamma = 0, \tag{4}$$

where g is a specified function of the coordinates and ρ is the net density of electron and ion space charge.

We assume that the magnetic field may be represented as the sum of the external magnetic field and the intrinsic magnetic field of the beam. The current $\mathbf{j}_e$ of the electron beam at the boundary where the particles enter the region is assumed to be either a known function of the coordinates, or is defined by the "3/2" law [4]. The ion current density $\mathbf{j}_i$ depends upon the parameters of the interaction between the electron beam and the neutral gas. The ions formed by collisions are assumed to be nonrelativistic. Their motion obeys the equation

$$Md^2\mathbf{R}_i/dt^2 = q\mathbf{E} + (e/c)[\mathbf{V}_i \times \mathbf{H}_e], \tag{5}$$

where M is the mass and q the charge of the ions, and $\mathbf{H}_e$ is the external magnetic field.

Calculation of the electric field, i.e., solution of Poisson equation (3) with boundary conditions (4), is performed by difference methods on a rectangular grid with piecewise-constant step [1].

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The external magnetic field is either homogeneous, or calculable throughout the region from values specified on the axis of symmetry with the aid of the series of [4]. For integration of the equations of motion (1) with initial conditions (2) we will use a scheme with second-order accuracy in time. In accordance with Bush's theorem [5] and using expressions for analytical extrapolation of the magnetic field from its values on the axis of symmetry, the angular velocity of an electron at the point (r, z) can be defined as [4]

$$\dot{\psi} = -\frac{e}{2m\gamma}\left[H(0, z) - \frac{r_0^2}{r^2}\left(H(0, z_0) - \frac{1}{8}r_0^2 H_z''(0, z_0)\right) - \frac{1}{8}r^2 H_z''(0, z)\right], \tag{6}$$

where (r_0, z_0) are the coordinates of the entry point. We introduce the quantities

$$p_r = \gamma v_r,\ p_z = \gamma v_z,\ p_\psi = \gamma\dot{\psi}$$

(where v_r, v_z are the components of the velocity $\mathbf{V}$).

From Eq. (1) we obtain the relationships

$$\frac{dp_r}{dt} = r\dot{\psi}^2\gamma + \frac{e}{m}E_r + \frac{e}{mc}\left(H_z r\dot{\psi} - H_\psi\frac{p_z}{\gamma}\right),$$
$$\frac{dp_z}{dt} = \frac{e}{m}E_z + \frac{e}{mc}\left(H_\psi\frac{p_r}{\gamma} - H_r r\dot{\psi}\right),$$

which we integrate numerically with step Δt_n using the scheme

$$p_r^{n+1} = p_r^n + \Delta t_n\left[r^{n+1/2}(p_\psi^{n+1/2})^2/\gamma^{n+1/2} + \frac{e}{m}E_r^{n+1/2} + \right.$$
$$\left. + \frac{e}{mc}(H_z^{n+1/2}r^{n+1/2}p_\psi^{n+1/2}/\gamma^{n+1/2} - H_\psi^{n+1/2}(p_z^n + p_z^{n+1})/(2\gamma^{n+1/2}))\right],$$
$$p_z^{n+1} = p_z^n + \Delta t_n\left[\frac{e}{m}E_z^{n+1/2} + \frac{e}{mc}(H_\psi^{n+1/2}(p_r^n + p_r^{n+1})/(2\gamma^{n+1/2}) - H_r^{n+1/2}r^{n+1/2}p_\psi^{n+1/2}/\gamma^{n+1/2}\right], \tag{7}$$

which has an error of $O(\Delta t_n^2)$.

The values of the electric and magnetic quantities are calculated here for the mean point

$$r^{n+1/2} = r^n + v_r^n\frac{\Delta t_n}{2},\ z^{n+1/2} = z^n + v_z^n\frac{\Delta t_n}{2}. \tag{8}$$

Near the axis of symmetry it may be the case that $r^{n+1/2} < 0$. In this case, the sign of the quantities r^n, $r^{n+1/2}$, v_r^n changes in Eq. (7). At the point with the coordinates of Eq. (8) we find the value $p_\psi^{n+1/2}$ with Eq. (6).

We carry out the final calculation of coordinates and velocities with the expressions

$$r^{n+1} = r^n + \frac{p_r^n + p_r^{n+1}}{2\gamma^{n+1/2}}\Delta t_n,\ z^{n+1} = z^n + \frac{p_z^n + p_z^{n+1}}{2\gamma^{n+1/2}}\Delta t_n,\ v_r^{n+1} = \frac{p_r^{n+1}}{\gamma^{n+1}},\ v_z^{n+1} = \frac{p_z^{n+1}}{\gamma^{n+1}},$$

where γ at the mean point is defined as

$$\gamma^{n+1/2} = 1 + \frac{|e\varphi(r^{n+1/2}, z^{n+1/2})|}{mc^2},$$

and at the (n + 1)-th point, as

$$\gamma^{n+1} = 1 + \frac{(p^{n+1})^2}{c^2},\ p^{n+1} = ((p_r^{n+1})^2 + (p_z^{n+1})^2 + (r^{n+1}p_\psi^{n+1})^2)^{1/2}.$$

Such an approach, i.e., calculation of γ at the mean point in terms of the potential, and at the (n + 1)-th point, in terms of the values of p_r^{n+1}, p_z^{n+1}, p_ψ^{n+1}, is used for the following reasons. Determination of the potential at any point requires a significant volume of calculations related to finding the closest-lying nodes of the difference grid and carrying out interpolation. At the point (n + 1/2) these operations are carried out in one way or the other during determination of the electric field intensity components, while at the point (n + 1) they must be performed specially just to determine γ. Therefore, in the latter case it is more economical to perform calculations with Eq. (9).

In calculating the intrinsic magnetic field we consider only the azimuthal component

$$H_\psi = 2I/cR,$$

where I is the current through a section of radius R.

The basis of the numerical algorithm for calculating H_ψ is the method described in [6]. Trajectories passing through nodes of the difference grid encompassing the subregion in which the beam travels recall the spatial pattern of current distribution I_{ij} in the region under consideration. In the present approach, commencing from the assumption that the current density is constant over the limits of the (i, j)-th elementary cell, the following expressions are constructed for calculation of the intrinsic magnetic field:

$$H_\psi(r_\tau, z_\tau) = \begin{cases} \dfrac{2I_{1j}}{c\left(0{,}5h_1^r\right)^2} r_\tau & \text{at } r_\tau \leqslant 0{,}5h_1^r, \\ \dfrac{2}{cr_\tau}\left[I_{i-1j} + (I_{ij} - I_{i-1j})\right]\dfrac{r_\tau^2 - r_{i-1/2}^2}{r_{i+1/2}^2 - r_{i-1/2}^2} & \text{at } r_\tau \geqslant 0{,}5h_1^r, \end{cases}$$

where $r_{i\pm1/2} = 0.5(r_i + r_{i\pm1})$; h_1^r is the grid step along the axis of symmetry; I_{ij} is the total current, i.e., the sum of the currents of all trajectories passing through the j-th section with area $\Delta S_{ij} = \pi(r_{i+1/2}^2 - r_{i-1/2}^2)$ [near the axis of symmetry $\Delta S_{ij} = 0.25\pi(h_1^r)^2$].

Numerical simulation of processes occurring upon passage of the electron beam through a medium with a residual gas is carried out in the following manner. We note that electrons generated in ionization processes are assumed to be "fast," and their contribution to the space charge is not considered.

In calculating the electron trajectory from the mean point (r_ξ^-, z_ξ^-) of each interval of length Δl_ξ^- we "release" an ion trajectory with initial conditions (7), carrying a current

$$\Delta I_{\nu\xi}^+ = I_\nu^- N_0 \sigma_i \Delta l_\xi^-,$$

where I_ν^- is the current of the electron trajectory, N_0 is the density of the neutral gas ($N_0 = p/kT$), σ_i is the ionization section, dependent on the electron energy [7]:

$$\sigma_i = c_1 \frac{\dfrac{\varphi\left(r_\xi^-, z_\xi^-\right)}{\varphi_i} - 1}{\left(\dfrac{\varphi\left(r_\xi^-, z_\xi^-\right)}{\varphi_I}\right)^2} \ln\left(1{,}25\frac{\varphi\left(r_\xi^-, z_\xi^-\right)}{\varphi_I}\right) \qquad (10)$$

(φ_I is the ionization potential and c_1 is a coefficient dependent on the characteristics of the residual gas). We integrate the equations of ion motion (5) numerically by a method of second-order accuracy. In calculating the ion trajectory, we will consider charge transfer processes, which consist of formation of a neutral and an ion. To do this, from the mean point (r_ξ^+, z_ξ^+) of each interval Δl_ξ^+ of the "primary" ion trajectory we "release" a secondary ion trajectory, carrying a current

$$\Delta I_{\nu\xi}^{+p} = \Delta I_{\nu\xi}^+ N_0 \sigma_{ip} \Delta l_\xi^+,$$

where σ_{ip} is the charge transfer section. This trajectory is calculated to its exit from the region without consideration of ionization processes caused by its ions. For further calculation of the "primary" ion trajectory, the current of the latter is decreased by the amount of the charge transfer current $\Delta I_{\nu\xi}^{+p}$. The section σ_{ip} is determined from the experimental dependence on primary beam energy.

The algorithms described above were realized in the form of a module for the ERA applications program package [1], written in FORTRAN. The package supports output of electron and ion trajectories to a plotter. Since the amount of data generated in problems with consideration of ionization effects is large, provision is made for dividing the calculation region into several subregions with output of ion trajectories in each such subregion to a specified resolution. This approach permits obtaining a detailed picture of trajectory behavior in the subregion of interest without the encumbrance of superfluous data output.

A calculation was performed for a one-dimensional planar diode $0 \leqslant z \leqslant z_k = 10$ cm with potential boundary conditions $\varphi(0) = 0$, $\varphi(z_k) = 500{,}00$ V, in which at the plane z = 0 an electron beam is released with zero initial velocity and current density calculable by the "3/2" law. The electron beam moves in an air medium under a pressure p = 0.667 Pa. Ionization of the residual gas, assumed to consist of nitrogen molecules, by electrons was considered.

The calculations were performed on a uniform grid with 80 steps along the z axis. The ion trajectories were "released" at intervals Δl_ξ^-, the lengths of which were determined as follows (dimensions in cm):

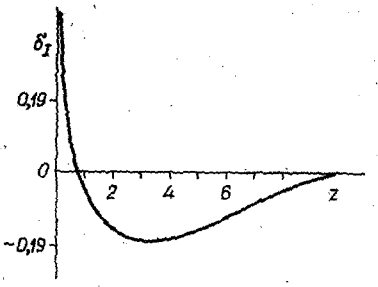

Fig. 1

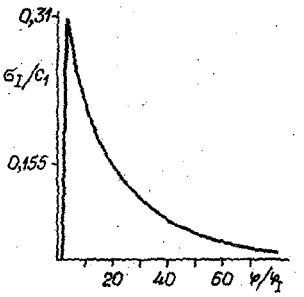

Fig. 2

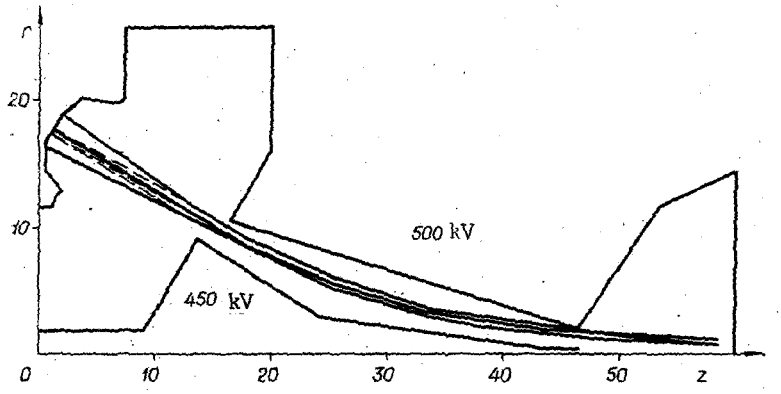

Fig. 3

$$\Delta\bar{l}_\xi = \begin{cases} 0.1 \text{ for } 0 \leqslant z \leqslant 0.5, \\ 0.25 \text{ for } 0.5 \leqslant z \leqslant 1.5, \\ 0.6 \text{ for } 1.5 \leqslant z \leqslant 10. \end{cases}$$

Figure 1 shows a graph of the function $\delta_I = (\varphi_p - \varphi_S)/\varphi_p$, the relative deviation of the potential distribution φ_p with consideration of ionization processes from the potential distribution φ_S of the self-consistent problem. This function is at a maximum in the cathode region, leading to a significant increase in density of the current removed from the cathode as compared to the self-consistent problem without consideration of ionization processes (the current density with consideration of ionization j_p = 18.1 A/cm^2, while with neglect of ionization j_S = 8.2 A/cm^2). This significant increase in current density causes the function to decrease and change sign upon exit from the cathode region.

Figure 2 shows the ionization section σ_i [$c_1 = 2 \cdot 10^{-15}$ cm^2 in Eq. (10)] as a function of potential; it is evident that this function also reaches its maximum near the cathode (the ionization potential of nitrogen molecules is equal to 15.6 eV).

To refine the calculations in the cathode region the following iteration process was developed. In the interval Ω_1 = [0, 0, 02] a higher-accuracy calculation was performed on a nonuniform grid with boundaries of the constant step zone $z_0 = 0$, $z_1 = 0.0005$, $z_2 = 0.001$, $z_3 = 0.002$, $z_4 = 0.004$, $z_5 = 0.009$, $z_6 = 0.02$ and number of nodes per zone $l_1 = 10$, $l_2 = 5$, $l_3 = 5$, $l_4 = 4$, $l_5 = 4$, $l_6 = 5$; the intervals $\Delta\bar{l}_\xi$ were then selected such that the electron trajectory traversed a distance between points at which the potential equalled $k_i\varphi_I$. The numbers k_i were specified as $k_1 = 1$, $k_2 = 1.5$, $k_3 = 2$, $k_4 = 2.5$, $k_5 = 3$, $k_6 = 5$, $k_7 = 6$, $k_8 = 8$, $k_9 = 10$, $k_{10} = 20$, $k_{11} = 30$, $k_{12} = 50$, $k_{13} = 100$, $k_{14} = 500$, $k_{15} = 2000$. On the subregion boundary at $z = 0.02$ the potential was specified from the solution of the same problem on the "coarse" grid. Using the current density obtained from the solution in this subregion, calculations were performed in the interval Ω_2 = [0.0156; 10] on a uniform grid with 100 nodes, and parameter $\Delta\bar{l}_\xi = 0.5$. The potential at the point $z = 0.0156$ was chosen from the solution in Ω_1. In obtaining the solution in Ω_2 the potential at the point $z = 0.02$ was recalculated by linear interpolation, the calculation was performed again in Ω_1, and so on, until the current density values in two successive iterations differed by no more than some small quantity. As a result of these calculations the current density proved equal to 28 A/cm^2, i.e., more than 50% larger than the current density obtained by calculations with the fixed grid, which indicates the need to perform more accurate calculations in the cathode region for such problems.

A practical problem proposed by P. I. Akimov was considered, involving calculation of an electron gun in an electron-optical system, the geometry of which is shown in Fig. 3. The pressure of the residual gas, assumed to consist of nitrogen molecules, was p = 0.667 Pa, with ionization section assumed constant for all energies ($\sigma_i = 3 \cdot 10^{-18}$ cm^2). The solid line of Fig. 3 shows the behavior of electron trajectories, while the dashed line is an example of ion trajectory behavior.

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VIBRATIONAL RELAXATION OF CO_2 MOLECULES DURING INJECTION INTO THE IONOSPHERE

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The problem of the influence of spacecraft flights on the state of the atmosphere is raised in connection with the active conquest of space. Spacecraft engines throw a large amount of H_2O, H_2, and CO_2 molecules into the atmosphere. The injected gas, in expanding, occupies volumes in the atmosphere with linear sizes of tens and even hundreds of kilometers. In this case the concentration of the ejected molecules remains comparable with the concentration of the atmospheric components. From this point of view, the injection of exhaust gases can make an appreciable contribution to the local heat balance of the atmosphere. The problem of the vibrational relaxation of water molecules behind a shock wave was discussed in [1] in connection with the above-indicated problem. The problem of the vibrational relaxation of CO_2 during mixing with the atmospheric gas is solved in the present work.

In the temperature range of 2000-3000°K the vibrational relaxation of CO_2 in collisions with molecules takes place more slowly than that of H_2O, while the rates of excitation of the vibrational degrees of freedom of CO_2 by electrons are considerably higher (by about 10^3). In the F region of the ionosphere the degree of ionization of the atmospheric gas reaches 10^{-3}, and hence electrons can play a definite role in the excitation of CO_2 vibrational levels, which in turn affects the thermal radiation.

Since the excitation of molecular gases by electrons is a natural phenomenon observed in the upper layers of the atmosphere, many papers have been devoted to this problem. A survey of papers on the rates of electron cooling in the ionosphere is made in [2], while [3] is devoted to the infrared emission of the undisturbed upper atmosphere with allowance for the excitation of CO_2 vibrational levels by electrons and the influence on the intensity of

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