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Boundary Conditions for Electron Balance Equation in the Stationary High-Frequency Induction Discharges

[1]Victor Semenovich Zheltuhin, [2]Pavel Sergeevich Solovyev and [2]Violetta Yurevna Chebakova
[1]Kazan State Technological University, Karl Marx Street 68, 420015 Kazan, Russia
[2]Federal University, Kremlevskaya Street 18, Volga District, 420008 Kazan, Russia

Abstract: The model of steady High-Frequency Induction (HFI) discharge of the reduced pressure provides the boundary problems for the diffusion equation of charged particles, the equations of heat conduction for electron and atomic-ion gas as well as the system of Maxwell equations describing the electromagnetic field distribution. In this research to solve the boundary value problem of electron balance in HFI discharge, a natural condition is considered where the diffusion flux of particles from the plasma coincides with the drift flux through the Layer of Positive Charge (LPC). It is established that this case is described by the boundary condition of the third kind. The model issues are solved numerically concerning the eigenvalues of the electron density obtaining with the condition as well as the problem with the condition of complete recombination of electrons on the walls of a gas discharge chamber. The effect of these conditions on the maximum value of the electron temperature is demonstrated. The mathematical justification of the maximum value dependence on the electron temperature from the smallest eigenvalue of the electron diffusion issue. We investigate the arising differences in the values of HFI discharge characteristics. It is established that the alleged condition describes the characteristics of the HFI discharge more adequately, in particular, it allows you to assess the discharge capacity more accurately as well as the electron drift velocity near the discharge chamber wall.

Key words: Mathematical modeling, inductive discharge, ambipolar diffusion, electron, electromagnetic field

INTRODUCTION

The High-Frequency Induction (HFI) discharge is widely used in various technological and plasma processes such as the treatment of textiles, leather and fur products (Abdullin *et al*., 2000; Mekeshkina-Abdullina and Kulevtsov, 2012), the accumulation of hydrogen with silicon powder (Kovalevsky *et al*., 2011), the synthesis of oxygen-free ceramics, the obtaining of carbide and boride materials for nuclear and manufacturing industries (Tumanov and Plasma, 2010).

The modes of material processing in these processes are extremely sensitive to the basic characteristics of HFI discharge. One of the most important parameters determining the plasma properties is plasma gas pressure. The technological processes use most commonly HFI discharge of atmospheric ($p \approx 0.1$ MPa) and low ($p \sim 10\text{-}3$ Pa) pressure. HFI-discharge of low ($13.3 \le p \le 133$ Pa) pressure is used much less frequently (Mekeshkina-Abdullina and Kulevtsov, 2012; Hubathuzin *et al*., 2013a, b).

HF plasma discharges of reduced pressure having all the advantages of high-frequency discharges has some specific properties inherent for the discharges at low pressures: a significant gap in the electron temperature from the ion one is the increased sterility of the environment, the ability to produce high temperature supersonic flows. In this regard, many techniques were developed concerning experimental measurements of induction plasma (Abdullin *et al*., 2000; Bolshakov and Kruden, 2008; Gainullin and Kirpichnikov, 2008). However, for more efficient and high-quality selection of design solutions at the creation of the HFI devices the creation of mathematical models is also necessary, as some of the plasma technological characteristics are not measured directly or such measurements are extremely time-consuming.

MATERIALS AND METHODS

Balance equation of charged particles: The model of steady HFI discharge of low pressure comprises the boundary-value problems for the diffusion equations of electrons, electron and atomic ion gas heat conduction equations and also the system of Maxwell's equations describing the electromagnetic field distribution.

Corresponding Author: Victor Semenovich Zheltuhin, Kazan State Technological University, Karl Marx Street 68, 420015 Kazan, Russia

Let's consider the boundary problem of the electron gas diffusion in detail. We assume that HFI discharge takes place in a cylindrical discharge chamber in which with the help of a system consisting of an ideal inductor, a high-frequency electromagnetic field is developed. The inductor idealness is that the current generated by it in the plasma is strictly circular one. Such an inducer creates a vortex electromagnetic field wherein the magnetic field is directed along the coil axis and the power lines of the electric field are concentric closed circles.

According to the provided suggestions, it may be assumed that a discharge has an axial symmetry. Therefore, during the direction of the coordinate axis perpendicular to an external electric field, the diffusion occurs in the cross direction of the field, the flow of charged particles of either sign is presented in the form usual for the diffusion flux. The estimates of elementary processes in the plasma of HFI low pressure discharges indicate that the mean free path length of atoms, ions and electrons, the Debye radius is much smaller than the radius of the discharge chamber (Abdullin *et al*., 2000) and therefore a violation of electrical neutrality may be neglected (Raiser, 2009) and the diffusion is ambipolar one. The time of stationary state is much larger than the period of the electromagnetic field oscillations. And, therefore, the fluctuation of plasma characteristics near the average for the period of value field change are negligible. Under these assumptions, the balance equation for the electrons in the plasma of HFI discharge of reduced pressure is the following one:

$$-\frac{1}{r}\frac{\partial}{\partial r}\left(rD_a\frac{\partial n}{\partial r}+rV_a n\right)=\nu_i n-\beta n^2 \quad \text{at} \quad 0<r<R \qquad (1)$$

Where:

R = Discharge chamber radius
D_a = The ambipolar diffusion coefficient
β = The coefficient of recombination
ν_i = Ionization frequency
V_a = Gas flow rate vector

The key dependences of the equation ratios may be seen (Raiser and Schneider, 1991; Hagelaar *et al*., 2005; Tkachev *et al*., 2007).

Boundary condition setting: We turn now to the formulation of the boundary conditions. The axis of the chamber symmetry is set with the condition $rD_a\,\partial n/\partial r \xrightarrow{r\to 0} 0$ which means a continuous flow. The discharge border with the surface of the Discharge Chamber (DC) the following condition is usually set $n_e|_{\Gamma=0}$, meaning the recombination of electrons on the walls of DC. However, this condition leads to an infinite value of the electron velocity $V_e = V_a - D_a/n_e \operatorname{grad} n_e - \mu_e E_{II}$ near DC wall which is contrary to the discharge physics. Here V_e is the macroscopic electron velocity vector, μ_e the electron mobility, E_{II} the potential component of the electric field stress vector.

It is known that near a solid surface in the plasma of any type an electric double (Debye) layer is developed and it acquires a negative potential relative to the plasma (floating potential):

$$\phi_b-\phi_p=V_f=-\left(\frac{kT_e}{2e}\right)\ln\left(\frac{m_i}{\gamma m_e}\right)$$

Where:

γ = $\gamma = 2\pi/e = 2.3$
e = The Euler number

Therefore instead of the full recombination term on the wall of DC, it is natural to consider the equation of charged particles balance under the condition of the particle diffusion flux equality and a drift flow through a double layer. The estimates of elementary processes in the plasma of low pressure high-frequency discharges indicate that the last collision is experienced by the particle at a distance of about one mean free path length l_e from the electrode surface. Under the reduced pressure of plasma gas the thickness of the double layer X_b is much less than the mean free path of electrons. Therefore, we assume that plasma is collisionless inside the double layer.

At first approximation, we assume that the deviation of the electron distribution function by energy is not essential from Maxwellian one. In this case, the electrode is covered only by the electrons the velocities of which are directed to the electrode surface and the energy of which is sufficient to overcome the potential barrier. Therefore, the microscopic density of electrons $\overline{\Gamma_e}\uparrow$ and ions $\overline{\Gamma_i}\uparrow$ on the surface may be presented as:

$$\overline{\Gamma_e}\uparrow=-\frac{n_b\overline{C_e}}{4}h_e,\quad \overline{\Gamma_i}\uparrow=-\frac{n_b\overline{C_i}}{4}h_i \qquad (2)$$

Where:

$\overline{C_{e,i}}=(8kT_{e,i}/\pi m_{e,i})^{1/2}$ = The average thermal velocity of the electrons and ions
n_b = The average thermal velocity of the electrons and ions, respectively the density of particles in the plasma and double layer boundary

The appearance of minus in Eq. 2 is related to the fact that the positive direction is given by the vector of normal to the sample surface h_e, h_i functions are determined as follows:

$$h_e = \begin{cases} \exp\left[\frac{e(\phi_b - \phi_p)}{kT_e}\right] & \text{npu } \phi_b \geq \phi_p \\ 1 & \text{npu } \phi_b \leq \phi_p \end{cases}$$
$$h_i = \begin{cases} \exp\left[\frac{e(\phi_b - \phi_p)}{kT_?}\right] & \text{npu } \phi_b \leq \phi_p \\ 1 & \text{npu } \phi_b \geq \phi_p \end{cases} \quad (3)$$

Where:

φ_b = The potential on the surface

φ_p = Plasma potential on the boundary of plasma and double layer (Mitchner and Kruger, 1976)

From the condition of particle flow continuity, it follows that the microscopic values defined by the ratio Eq. 4 and 5 shall be equal to the corresponding flux density flows at x = X_b:

$$U_e = -\frac{\mu_e}{\mu_e + \mu_i}\frac{J_b}{en_b} - \frac{D_a}{n_b}\left(\frac{dn}{dx}\right)_b$$
$$U_i = -\frac{\mu_i}{\mu_e + \mu_i}\frac{J_b}{en_b} - \frac{D_a}{n_b}\left(\frac{dn}{dx}\right)_b \quad (4)$$

Thus, we obtain the following system:

$$\begin{cases} -\frac{n_b\overline{C_e}}{4}h_e = -\frac{\mu_e}{\mu_e + \mu_i}\frac{J_b}{en_b} - \frac{D_a}{n_b}\left(\frac{dn}{dx}\right)_b \\ -\frac{n_b\overline{C_i}}{4}h_i = -\frac{\mu_i}{\mu_e + \mu_i}\frac{J_b}{en_b} - \frac{D_a}{n_b}\left(\frac{dn}{dx}\right)_b \end{cases} \quad (5)$$

Dividing the first equation of the system by μ_e, the second one by μ_i and adding them, we obtain the following boundary condition:

$$D_a\left(\frac{dn}{dx}\right)_b = n_b\left(\frac{\mu_i\overline{C_e}h_e + \mu_e\overline{C_i}h_i}{4(\mu_e + \mu_i)}\right) \quad (6)$$

Now, let's determine $\phi_p - \phi_b = \overline{V_p}$, the potential difference between the plasma boundary and the surface required for the calculation of $h_{e,i}$.

Let's consider the surface as the electrode with the instantaneous value of the potential relative to plasma (the lower limit of the ambipolar field) equal to V_p. Then the constant plasma potential relative to the electrode $\overline{V_p}$ is obtained by averaging the instantaneous voltage drop in the layer according to the oscillation period, it makes $\overline{V_p} = 3\pi en_{eb}A^2$ (Raiser *et al.*, 1995) where A the vibrational motion of electrons displacement, equal to the thickness of SPZ:

$$A = \left(\frac{8}{9}\right)^{1/2}\left(e\frac{\overline{V_p}}{kT_e}\right)^{3/4}\left(\frac{kTe}{4\pi e^2 n}\right)^{1/2} \quad (7)$$

Thus, we obtain $\phi_p - \phi_b = \overline{V_p} = \frac{9kTe}{4e}$.

Mathematic justification: The problem of balance concerning HFI discharge of charged particles is a non-linear problem on eigenvalues, although an explicit spectral parameter is missing. In order to explain the origin and nature of the spectral parameter, let's consider the linear problem:

$$-\frac{1}{r}\frac{\partial}{\partial r}\left(rD_a\frac{\partial n}{\partial r} + rV_a n\right) = \nu_i n, \quad 0 < r < R \quad (8)$$

We carry out the change of variables as scaling factors of parameter values at the point r^* on the discharge axis which attains the maximum concentration of electrons:

$$n^* = n(r^*), T_e^* = T_e(r^*), D_a^* = D_a(T_e^*), \nu_i^* = \nu_i(T_e^*)$$

The result of variables change is presented as follows:

$$-\frac{1}{\bar{r}}\frac{\partial}{\partial \bar{r}}\left(\bar{r}\overline{D_a}\frac{\partial \bar{n}}{\partial \bar{r}} + \bar{r}\overline{V_a n}\right) = l_0^2\overline{\nu_i n}, \quad 0 < \bar{r} < 1 \quad (9)$$

Where:

$$l_0^2 = \frac{\nu_i^*\left(T_e^*\right)R^2}{D_a^*(T_e^*)}$$

The boundary conditions at such a change take the following form:

$$\frac{\overline{D_a}D_a^*}{R}\left(\frac{\partial \bar{n}}{\partial \bar{r}}\right) = \bar{n}\left(\frac{\mu_+\bar{\upsilon}_e h_e + \mu_e\bar{\upsilon}_+ h_+}{4(\mu_+ + \mu_e)}\right) \text{ at } \bar{r} = 1$$
$$\bar{r}\overline{D_a}\frac{\partial \bar{n}}{\partial \bar{r}} \xrightarrow{\bar{r} \to 0} 0 \quad (9)$$

On the axis of symmetry. Thus, the considered linear problem after this change of variables is the task on its own values with a spectral parameter l_0^2. The eigenvalues of the problem form an infinite discrete spectrum, so the question arises, what is the own value as the solution? The answer to it may be found, if you start from the physical meaning of the variable $\bar{n}$. The concentration of the substance can not be a negative one, hence the physical sense has only a non-negative eigenfunction of the issue. According to the theory of eigenvalue problems, it is known that a non-negative eigenfunction corresponds to the smallest eigenvalue. Therefore to solve the problem, you need to find the smallest eigenvalue and the corresponding eigen function.

Since, the eigenvalues of the differential problem is entirely determined by the coefficients of the equation and the boundary conditions, the only free parameter in the scaled problem is the value of the electron temperature in the center of the discharge T_e^* which satisfies a certain relation between the coefficient of ambipolar diffusion, the rate of ionization, the recombination coefficient and the radius of the plasmatron. This relationship defines a necessary condition necessary to maintain the stationary HFI discharge of low pressure.

It is obvious that similar to the linear case, the eigenvalues of the nonlinear problem are also the function of the electron temperature but the condition for its determination can not be written in an analytical form.

The conditions for the existence of a minimum eigenvalue corresponding to positive eigenfunction of a nonlinear problem on eigenvalues with the coefficients depending on the spectral parameter for finding the concentration of charged particles for a steady HFI discharge are established (Zheltukhin *et al*., 2014). During the solution of nonlinear stationary problems (Fedorenko, 2014; Badriev and Karchevskii, 1994; Badriev *et al*., 2014) and non stationary problems (Badriev and Banderov, 2004; Solovev, 2010, 2011, 2012, 2013), you may use the methods proposed by Solovev (2011, 2012, 2013).

RESULTS AND DISCUSSION

Analysis of numerical calculation results: The mathematical model that takes into account the processes discussed in this study was implemented numerically. The comparison of numerical calculation results concerning the solutions of boundary model problems with both the equality condition to zero concentration (the condition of the first kind) on the walls of a discharge chamber and with the condition (Eq. 6) (of the third kind) with the help of numerical simulation. Both problems are nonlinear eigenvalue problems, the spectral parameter of which, due to the dependencies D_a and μ_i from T_e is the maximum value of the electron temperature T_e^*. It was established that the distributions $\bar{n}(x)$, normalized to unity when using the boundary condition of the first kind and the boundary condition and the third kind differ substantially only near the boundary of a discharge gas chamber (Fig. 1). But the value T_e^*, obtained as the resulting solution of the problem with the boundary condition of the third kind is much less than the value T_e^*, obtained as the result of the problem solution with the condition of the first kind (Fig. 2).

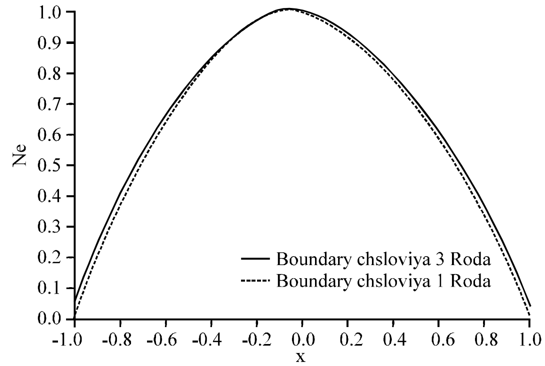

Fig. 1: The distribution of $\bar{n}(x)$ in the area between electrodes at different boundary conditions

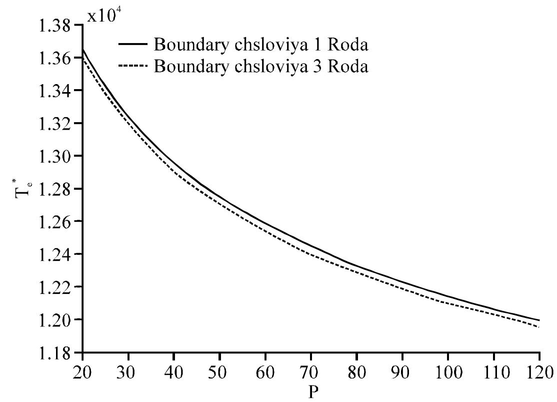

Fig. 2: Dependences of the electron temperature necessary to maintain the discharge pressure

Summary: The boundary condition on the wall of a discharge gas chamber, delivered for the concentration of charged particles under the equality assumption concerning the diffusion flux of particles from plasma and a drift flow through SPPZ, due to the model non-linearity has a significant effect on the maximum temperature in the electrode gap which leads to inaccurate estimates of characteristics and discharge parameters.

CONCLUSION

The boundary condition set on the wall of the DC has a more significant effect on the maximum value of the electron temperature in the electrode gap than on the charged particle concentration distribution. This is due to the nonlinearity of a HFI discharge mathematical model and the spectral parameter dependence on the electron temperature which in its turn may be represented as an implicitly given function from the smallest eigenvalue.

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