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Boundary conditions in fluid models of gas discharges

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Fluid models of gas discharges are typically based on continuity equations and drift-diffusion equations for plasma particle species. The boundary conditions for these equations are an important part of the description of the problem. In this Brief Report, we point out that the most commonly used boundary conditions do not describe the physics properly. We present improved boundary conditions that can be used instead.

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Fluid models are widely used in gas discharge physics. All these models are based on the first few moments of the Boltzmann equation, i.e., balance equations for mass, momentum, and energy. For every species, the particle density n is calculated from a continuity equation

$$\frac{\partial n}{\partial t}+\boldsymbol{\nabla}\cdot\boldsymbol{\Gamma}=S, \tag{1}$$

where $\boldsymbol{\Gamma}$ is the particle flux and S the particle source term, resulting from reactions taking place in the plasma. The flux is given by the momentum transport equation, which is typically approximated by the drift-diffusion equation

$$\boldsymbol{\Gamma}=\mathrm{sgn}(q)\mu\mathbf{E}n-D\boldsymbol{\nabla}n, \tag{2}$$

where $\mathbf{E}$ is the electric field and q the particle charge. The mobility μ and the diffusion coefficient D are input parameters. The diffusion coefficient is usually found from the mobility by the Einstein relation

$$D=\frac{k_BT\mu}{e}, \tag{3}$$

where k_B is the Boltzmann constant, e is the elementary charge, and T is the particle temperature, corresponding to the energy of the random particle motion. For ions, μ, D, and T are generally treated as functions of the electric-field strength. Often semi-empirical formulas are used, for instance, for the ion temperature [1]:

$$k_BT=k_BT_g+\frac{m+m_g}{5m+3m_g}m_g(\mu E)^2, \tag{4}$$

where T_g is the gas temperature, E is the magnitude of the electric field, and m and m_g are the ion and gas particle masses, respectively.

The boundary conditions for the above transport equations are an essential part of the description of the problem. A variety of them can be found in the literature. Straightforward boundary conditions, such as $n=0$ or $\boldsymbol{\nabla}n\cdot\mathbf{n}=0$, with $\mathbf{n}$ a normal vector, are satisfactory in some cases [2–5], but do generally fail to fit the physics. In particular, the physical phenomenon of secondary electron emission by the surface, which is essential for many types of discharges, is not described by these conditions. Most authors therefore use a more general approach, imposing expressions for the particle fluxes, which for electrons may include secondary-electron emission. For instance, Refs. [6–10] assume the flux to be directed toward the surface according to

$$\boldsymbol{\Gamma}\cdot\mathbf{n}=a\,\mathrm{sgn}(q)\mu\mathbf{E}\cdot\mathbf{n}n+\tfrac{1}{4}v_{\mathrm{th}}n, \tag{5}$$

where $\mathbf{n}$ is the normal vector pointing toward the wall and v_{th} is the thermal velocity:

$$v_{\mathrm{th}}=\sqrt{8k_BT/\pi m}. \tag{6}$$

The number a is set to one if the drift velocity is directed toward the wall and to zero otherwise:

$$a=\begin{cases}1, & \mathrm{sgn}(q)\mu\mathbf{E}\cdot\mathbf{n}>0\\ 0, & \mathrm{sgn}(q)\mu\mathbf{E}\cdot\mathbf{n}\leqslant 0.\end{cases} \tag{7}$$

In the case of electrons, a flux due to secondary emission is added to the flux defined by Eq. (5):

$$\boldsymbol{\Gamma}_e\cdot\mathbf{n}=-a_e\mu_e\mathbf{E}\cdot\mathbf{n}n_e+\tfrac{1}{4}v_{\mathrm{th},e}n_e-\sum_p\gamma_p\boldsymbol{\Gamma}_p\cdot\mathbf{n}, \tag{8}$$

where the subscript e refers to electrons, and the summation in the last term is over the ion species impinging on the wall. The secondary emission coefficient γ is the average number of electrons emitted per incident ion.

In this Brief Report, we will show, however, that the boundary conditions (5) and (8) fall short of physical reality in several ways. We will propose improved boundary conditions that can be used instead.

To start with, we discuss the particle flux toward the wall. From kinetic considerations, it follows that under drift-diffusion conditions, the particle flux toward the wall is given by [11,12]

$$\boldsymbol{\Gamma}\cdot\mathbf{n}=(1-r)\ \left[a\,\mathrm{sgn}(q)\mu\mathbf{E}\cdot\mathbf{n}n+\tfrac{1}{4}v_{\mathrm{th}}n-\tfrac{1}{2}D\boldsymbol{\nabla}n\cdot\mathbf{n}\right], \tag{9}$$

where r is the fraction of particles reflected by the surface, and a is once again given by Eq. (7). The last two terms represent the diffusion flux, due to the random motion of the particles. The last term, which is wrongly ignored in many papers, e.g., in the boundary condition (5), reflects the fact that this random motion flux involves all particles within a certain mean free path from the wall, not just the local particles at the wall. In order to circumvent possible numerical difficulties in accurately evaluating the density gradient in this term, we will now rewrite Eq. (9). Imposition of the expression (9) as a boundary condition for the drift-diffusion equation (2) implies that the following equation must hold at the boundary:

$$\sin(q)\mu\mathbf{E}\cdot\mathbf{n}n - D\boldsymbol{\nabla}n\cdot\mathbf{n} = (1-r)[a\sin(q)\mu\mathbf{E}\cdot\mathbf{n}n + \tfrac{1}{4}v_{\mathrm{th}}n - \tfrac{1}{2}D\boldsymbol{\nabla}n\cdot\mathbf{n}]. \tag{10}$$

Note that although both members of this equation contain similar terms, their nature is very different: the left member is a continuum expression, which, in principle, can be used anywhere in space, but only has physical meaning inside the plasma volume, whereas the right member is a kinetic expression for the flux at the boundary. From Eq. (10), we find an expression to replace the last term in Eq. (9). Substitution of that expression gives

$$\boldsymbol{\Gamma}\cdot\mathbf{n} = \frac{1-r}{1+r}[(2a-1)\mathrm{sgn}(q)\mu\mathbf{E}\cdot\mathbf{n}n + \tfrac{1}{2}v_{\mathrm{th}}n]. \tag{11}$$

This equation is an appropriate boundary condition for heavy-particle species. It has the same structure as the usual condition (5), but gives a better physical description. For neutral species ($\mu=0$), Eq. (11) corresponds to the diffusion boundary condition derived by Chantry, using the concept of ''linear extrapolation length'' [13]. In the case of electrons, influx due to secondary electron emission must be taken into account. Simple addition of this influx to the flux toward the wall, as is done in equation (8), gives

$$\boldsymbol{\Gamma}_e\cdot\mathbf{n} = (1-r_e)\ [-a\mu_e\mathbf{E}\cdot\mathbf{n}n_e + \tfrac{1}{4}v_{\mathrm{th},e}n_e - \tfrac{1}{2}D_e\boldsymbol{\nabla}n_e\cdot\mathbf{n}] - \sum_p \gamma_p\boldsymbol{\Gamma}_p\cdot\mathbf{n}. \tag{12}$$

Equating the drift-diffusion flux, as before, Eq. (12) becomes

$$\boldsymbol{\Gamma}_e\cdot\mathbf{n} = \frac{1-r_e}{1+r_e}[-(2a_e-1)\mu_e\mathbf{E}\cdot\mathbf{n}n_e + \tfrac{1}{2}v_{\mathrm{th},e}n_e] - \frac{2}{1+r_e}\sum_{\mathbf{p}} \gamma_p\boldsymbol{\Gamma}_p\cdot\mathbf{n}. \tag{13}$$

This boundary condition is our counterpart of the common electron condition (8). However, as we point out now, both of these boundary conditions lead to an unrealistic artifact: According to these conditions, *all* electrons in front of the surface contribute to the diffusion flux toward the wall, including the electrons emitted by secondary emission. In this way, the diffusion terms in Eqs. (8) and (13) introduce an overaccounting of the backscattering of emitted electrons: Several studies [14,15] have demonstrated that in reality, virtually no emitted electrons are scattered back to the surface if a high enough electric field ($>100\ \mathrm{V\,cm^{-1}\,Torr^{-1}}$) is present, as is typically the case in front of cathode surfaces.

In order to find a more realistic boundary condition for electrons, we distinguish between two electron groups at the wall: α electrons, coming from the bulk, and γ electrons, emitted by the surface. Both groups are treated equally and indistinguishably with the drift-diffusion equation, but have different boundary conditions. To the α electrons, we apply the boundary condition (11):

$$\boldsymbol{\Gamma}_\alpha\cdot\mathbf{n} = \frac{1-r_e}{1+r_e}[-(2a_e-1)\mu_e\mathbf{E}\cdot\mathbf{n}n_\alpha + \tfrac{1}{2}v_{\mathrm{th},e}n_\alpha], \tag{14}$$

where $\boldsymbol{\Gamma}_\alpha$ and n_α are the flux and density of the α electrons. In contrast, the γ electrons do not flow (back) to the wall:

$$\boldsymbol{\Gamma}_\gamma\cdot\mathbf{n} = -(1-a_e)\sum_{\mathbf{p}} \gamma_p\boldsymbol{\Gamma}_p\cdot\mathbf{n}, \tag{15}$$

where $\boldsymbol{\Gamma}_\gamma$ is the flux of γ electrons, and the factor $(1-a_e)$ is included to cancel the flux in case the electric field is directed away from the wall. The sum of the two fluxes (14) and (15) can be used as a boundary condition for the total electron flux, if we manage to relate the density of the α electrons in Eq. (14) to the total electron density. Keeping in mind that $n_\alpha = n_e - n_\gamma$, where n_γ is the density of the γ electrons, we choose the following approach.

We write expression (15) as the boundary condition for the drift-diffusion equation for γ electrons, in analogy to Eq. (10):

$$-\mu_e\mathbf{E}\cdot\mathbf{n}n_\gamma - D_e\boldsymbol{\nabla}n_\gamma\cdot\mathbf{n} = -(1-a_e)\sum_{\mathbf{p}} \gamma_p\boldsymbol{\Gamma}_p\cdot\mathbf{n}. \tag{16}$$

Secondary-electron emission is important mainly where a strong electric field is directed toward the wall. In this case it is justified to neglect the second term in the left member of this equation, which gives us the density of the γ electrons:

$$n_\gamma = (1-a_e)\frac{\sum_p \gamma_p\boldsymbol{\Gamma}_p\mathbf{n}}{\mu_e\mathbf{E}\cdot\mathbf{n}}. \tag{17}$$

Note that this expression may be incorrect if the electric field is small, but in that case n_γ is negligible anyway ($n_\alpha \approx n_e$). Realizing that the ion fluxes $\boldsymbol{\Gamma}_p$ are largely proportional to $\mathbf{E}$ we find that

$$n_\gamma \approx (1-a_e)\frac{1}{\mu_e}\sum_p \gamma_p\frac{1-r_p}{1+r_p}\left[(2a_p-1)\mathrm{sgn}(q_p) + \frac{1}{2}\left(\frac{8}{\pi}\frac{(m_p+m_g)}{(5m_p+3m_g)}\frac{m_g}{m_p}\right)^{1/2}\right]\mu_p n_p. \tag{18}$$

For this approximation, we used Eqs. (11), (6), and (4), where we neglected the gas temperature and assumed the electric field to be perpendicular to the wall.

Finally, we obtain the appropriate boundary condition for the total electron flux, by adding the fluxes (14) and (15) of the two electron groups, and substituting $n_\alpha = n_e - n_\gamma$ and expression (17):

$$\boldsymbol{\Gamma}_e\cdot\mathbf{n} = \frac{1-r_e}{1+r_e}[-(2a_e-1)\mu_e\mathbf{E}\cdot\mathbf{n}n_e + \tfrac{1}{2}v_{\mathrm{th},e}n_e - \tfrac{1}{2}v_{\mathrm{th},e}n_\gamma] - \frac{2}{1+r_e}(1-a_e)\sum_p \gamma_p\boldsymbol{\Gamma}_p\cdot\mathbf{n}, \tag{19}$$

where n_γ is once again given by Eq. (17) or by the numerically more convenient expression (18). This boundary condition is similar to the boundary condition (13), except for

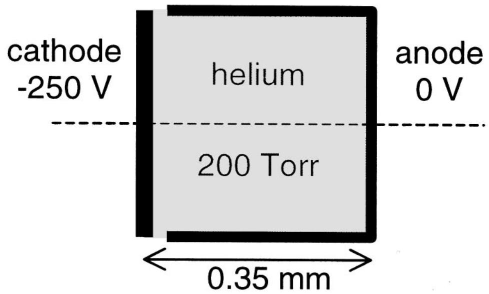

FIG. 1. Two-dimensional Cartesian dc discharge geometry used for the test calculations.

the term containing n_γ, which provides a correction for the directed motion of the emitted electrons. Due to this term, the boundary condition automatically switches between the limit (15) for high fields toward the wall, and the limit (14) for low fields or fields directed from the wall.

In order to demonstrate the effect of the correction term, we simulated a dc discharge in an imaginary two-dimensional rectangular geometry, with one cathode wall and three anode walls. The geometry is represented in Fig. 1. The discharge gas is helium; only two particle species are taken into account, electrons and helium ions. The secondary-emission coefficient of the ions is assumed to be $\gamma=0.20$. We calculated the steady-state solution of the transport equations, using Eq. (19) as the boundary condition for electrons. It turned out that the correction term almost entirely canceled the diffusion flux (back) toward the cathode: $n_\gamma>0.98n_e$ all over the cathode surface, so that $\mathbf{\Gamma}_e\cdot\mathbf{n}\approx\mathbf{\Gamma}_\gamma\cdot\mathbf{n}$. At the anode, on the other hand, the correction term was of minor importance: $n_\gamma<0.1n_e$, which means that nearly all electrons contributed to the diffusion component. We did the same calculation without the correction term, setting $n_\gamma=0$ everywhere. In this case, we found that the electron influx due to secondary emission from the cathode was partially canceled by diffusion back to the surface, so that $\mathbf{\Gamma}_e\cdot\mathbf{n}\approx0.7\mathbf{\Gamma}_\gamma\cdot\mathbf{n}$ at the cathode. As a result, the steady-state plasma density was about one order of magnitude lower. This dramatic effect is illustrated by Fig. 2, which

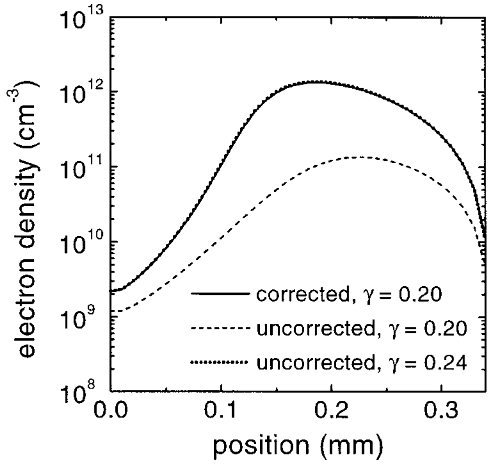

FIG. 2. Calculated steady-state electron densities along the dashed line in the geometry of Fig. 1. The cathode and anode are at the left- and right-hand side of the picture, respectively. The figure compares the boundary condition (19), including a correction term for the directed motion of emitted electrons, to the same boundary condition without the correction term.

shows the calculated steady-state electron density for the two cases. It turned out that the unrealistic backscattering flux toward the cathode can be compensated for by artificially increasing the secondary-emission coefficient. Using $\gamma=0.24$ instead of $\gamma=0.20$ led to virtually the same plasma density as the corrected boundary condition.

In conclusion, we have pointed out some shortcomings of the commonly used boundary conditions (5) and (8): First, the diffusion flux to the surface is only partially included. Second, the treatment of secondary-electron emission may lead to an unrealistic diffusion flux of emitted electrons back to wall. This artifact necessitates the use of unphysically high secondary-emission coefficients. We have presented alternative boundary conditions, where these problems have been solved in an elegant way.

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[1] H. W. Ellis, R. Y. Pai, E. W. McDaniel, E. A. Mason, and L. A. Viehland, At. Data Nucl. Data Tables **17**, 177 (1976).
[2] M. Meyyappan and J. P. Kresovsky, J. Appl. Phys. **68**, 1506 (1990).
[3] M. Surendra, D. B. Graves, and G. M. Jellum, Phys. Rev. A **41**, 1112 (1990).
[4] J. D. P. Passchier and W. J. Goedheer, J. Appl. Phys. **74**, 3744 (1993).
[5] K. C. Choi and K.-W. Whang, IEEE Trans. Plasma Sci. **23**, 399 (1995).
[6] J. Meunier, Ph. Belenguer, and J. P. Boeuf, J. Appl. Phys. **78**, 731 (1995).
[7] J. P. Boeuf and L. C. Pitchford, Phys. Rev. E **51**, 1376 (1995).
[8] C. Punset, J.-P. Boeuf, and L. C. Pitchford, J. Appl. Phys. **83**, 1884 (1998).
[9] V. V. Ivanov, Yu. A. Mankelevich, O. V. Proshina, A. T. Rakhimova, and T. V. Rakhimova, Plasma Phys. Rep. **25**, 591 (1999).
[10] R. Veerasingam, R. B. Campbell, and R. T. McGrath, Plasma Sources Sci. Technol. **6**, 157 (1997).
[11] E. W. McDaniel, *Collision Phenomena in Ionized Gases* (Wiley, New York, 1964).
[12] R. R. Newton, Phys. Rev. **73**, 570 (1948).
[13] P. J. Chantry, J. Appl. Phys. **62**, 1141 (1987).
[14] V. P. Nagorny and P. J. Drallos, Plasma Sources Sci. Technol. **6**, 212 (1997).
[15] A. V. Phelps and Z. Lj. Petrovic, Plasma Sources Sci. Technol. **8**, R21 (1999).