Implicit, approximately-factored, upwind scheme for glow discharge modeling

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Abstract

A three-dimensional computer code has been written to solve the drift-diffusion equations and the Poisson equation in an implicit, loosely-coupled fashion. Exploratory calculations have been carried out for nitrogen discharges between parallel plates. Several numerical techniques, including proper evaluation of source terms and implicit procedures, were critical to successful, high-fidelity simulations. Issues of numerical stability in modeling the juncture between an insulator and conductor have been investigated. Adequate grid resolution and a robust numerical scheme were found to be necessary to accurately capture this phenomenon.

Keywords: DC Glow discharge; Numerical methods; Finite-difference; Insulator/conductor juncture

1. Introduction

Plasma actuators are currently considered to be a promising means of flow control. Accurate simulation of such flow control devices requires modeling many physical phenomena which are not incorporated into conventional fluid dynamics codes, particularly space charge effects or sheaths. The present work is aimed at developing a capability to simulate experiments with plasma actuators, and a computer code has been written in order to model flow in the presence of finite space charge effects and to examine the sheaths present near electrode surfaces[1]. In the present paper, calculations of DC glow discharges in nitrogen have been carried out for a discharge between parallel plates, and issues of numerical stability in modeling the juncture between an insulator and conductor have been investigated.

2. Methodology

Although the computer code PS3D developed in this project has extended capabilities, including the effects of bulk fluid flow and an applied magnetic field, here we describe only the model relevant to the work presented in this paper.

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2.1 Physical model

Neglecting acceleration terms and diffusion due to temperature gradients, the particle and momentum conservation equations for each species can be combined to obtain a drift-diffusion model:

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (s_s n_s \mu_s \mathbf{E}) = \nabla \cdot (D_s \nabla n_s) + \omega_s \tag{1}$$

where $s_s = \pm 1$ is the sign of the charge on species s. Only two species (positive ions and electrons) are considered in the present work.

For the present work, the charged particle generation rate is taken to have the form:

$$\omega_{i,e} = \alpha \Gamma_e - \beta n_i n_e \tag{2}$$

where α is the ionization coefficient, β is the recombination coefficient, and Γ_e is the magnitude of the electron flux. All the calculations presented in this paper were carried out for nitrogen gas. Data for the mobilities, diffusion coefficients, ionization coefficient, and recombination coefficient were taken from [2].

The electric potential is determined from the Poisson equation:

$$\nabla^2 \phi = -\zeta / \epsilon_0 \tag{3}$$

where ϵ_0 is the permittivity of free space. The electric field is found from $\mathbf{E} = -\nabla \phi$.

The ion number density at the anode was determined by assuming a zero normal component of the ion current there, and the electron number density on the cathode was found from the relation:

$$\boldsymbol{\Gamma}_e \cdot \mathbf{n} = -\gamma \boldsymbol{\Gamma}_i \cdot \mathbf{n} \tag{4}$$

where γ is the secondary emission coefficient, $\mathbf{n}$ is a unit normal vector, and $\boldsymbol{\Gamma}_{i,e}$ are the species fluxes.

The potential at the anode was taken to be zero. The cathode potential V_c was determined according to $V_c = -V + IR$, where V is the applied voltage in the external circuit, R is the corresponding resistance, and I is the total current at the anode.

2.2 Numerical method

The drift-diffusion equations (1) and Poisson equation (3) are solved in a loosely-coupled, subiteration procedure.

The drift-diffusion equations are solved using an approximately factored, implicit, upwind scheme. Writing the governing equations (1) in conservation form, then applying the standard transformation from physical coordinates (x, y, z) to grid coordinates (ξ, η, ζ), gives:

$$\frac{\partial \bar{U}}{\partial t} + \frac{\partial \bar{E}}{\partial \xi} + \frac{\partial \bar{F}}{\partial \eta} + \frac{\partial \bar{G}}{\partial \zeta} = \frac{\partial \bar{E}_v}{\partial \xi} + \frac{\partial \bar{F}_v}{\partial \eta} + \frac{\partial \bar{G}_v}{\partial \zeta} + \bar{S} \tag{5}$$

We introduce subiterations such that $\bar{\mathrm{U}}^{n+1} \to \bar{\mathrm{U}}^{p+1}$, with $\Delta\bar{\mathrm{U}} = \bar{\mathrm{U}}^{p+1} - \bar{\mathrm{U}}^{p}$. Writing Eq. (5) as $\partial\bar{\mathrm{U}}/\partial t = R$, the right-hand side R^{n+1} is linearized in the standard thin layer manner. Collecting the implicit terms on the left-hand side, and introducing approximate factoring and a subiteration time step $\Delta\hat{t}$ gives an equation of the form:

$$L_\xi L_\eta L_\zeta \Delta \bar{U} = -\frac{\Delta \hat{t}}{1+\theta} \left\{ \frac{(1+\theta)\bar{U}^p - (1+2\theta)\bar{U}^n + \theta \bar{U}^{n-1}}{\Delta t} - R^p \right\} \tag{6}$$

where the operators on the left-hand side consist of derivative operators and flux and source Jacobian terms. These equations are discretized in space using a second-order upwind scheme based on the drift velocity. The minmod limiter is employed. An upwind method is also applied when calculating the species fluxes present in the source terms [2].

The Poisson equation is solved using an approximately factored implicit scheme, adapted from the approach described by Holst [3]. Applying the transformation of coordinates, and introducing an artificial time term, Eq. (3) can be written in the form:

$$\frac{\partial \phi}{\partial \tau} = L\phi = \frac{\partial \bar{E}}{\partial \xi} + \frac{\partial \bar{F}}{\partial \eta} + \frac{\partial \bar{G}}{\partial \zeta} - \bar{S} \tag{7}$$

We apply a procedure that drives the numerical solution towards $L\phi = 0$. We write $\Delta\phi/\Delta\tau = L\phi^{p+1}$, where $\Delta\phi = \phi^{p+1} - \phi^{p}$. We linearize the right-hand side using the standard thin-layer approach, then introduce an over-relaxation parameter ω and approximate factoring. This gives:

$$L_\xi L_\eta L_\zeta \Delta\phi = \omega \Delta\tau L \phi^p \tag{8}$$

The spatial derivatives are evaluated using second-order central differences. In order to accelerate convergence, the pseudo-time parameter is varied cyclically.

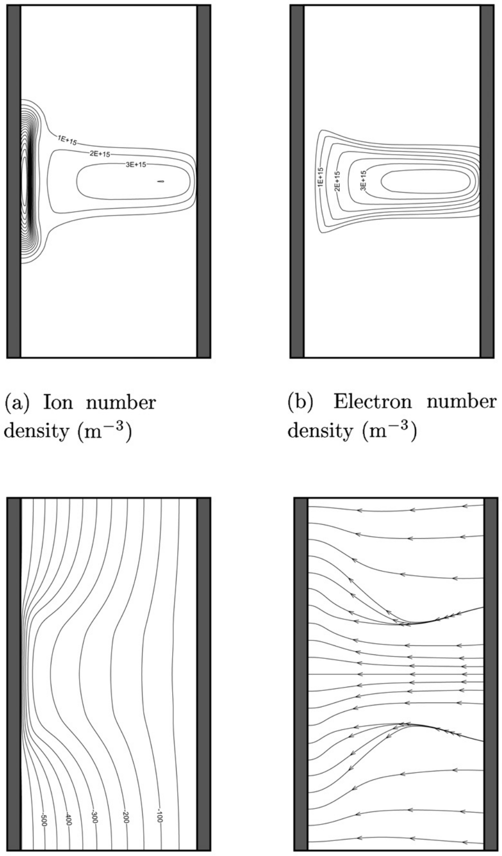
3. Results and conclusions

A set of calculations was carried out for a simple discharge between parallel plates. A grid of 61 × 141 × 5 points, clustered near the electrodes and the symmetry plane, was used on a 20 mm × 40 mm × 10 mm domain. Uniformity was imposed in the z-direction for all variables.

Contour plots of selected discharge properties for a case in the normal glow regime are shown in Fig. 1. The electrodes are indicated as vertical shaded bars just outside the computational domain. The results illustrate the normal glow behavior: the column of ionized gas carrying the discharge current occupies only a portion of the electrode surfaces. The cathode layer is characterized by a large potential drop and an ion number density that is an order of magnitude above that in the positive column.

For the case shown in Fig. 2, all the parameters are the same, but the extent of the electrodes along the y-direction has been reduced. A shaded region again indicates the position of the electrodes, and insulated regions are indicated by a white box. A strong peak in the ion number density is again seen at the cathode, whereas the character of the solution near the anode has strongly changed with the presence of finite electrodes. Strong peaks in the number densities of both ions and electrons occur near the edges of the anode, and much of the current originates from these edges and flows to the cathode.

In summary, a three-dimensional computer code has been written to solve the drift-diffusion equations and the Poisson equation in an implicit, loosely-coupled fashion, and exploratory calculations of DC glow discharges in nitrogen have been carried out for a parallel plate configuration. Adequate grid resolution and a robust numerical scheme were found to be necessary to accurately capture phenomena occuring near electrode/insulator junctures.



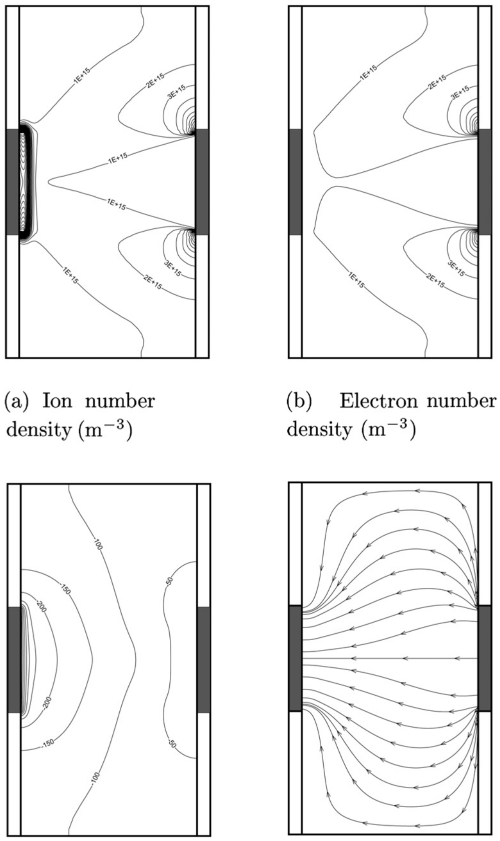
(a) Ion number density (m^{-3})

(b) Electron number density (m^{-3})

(c) Potential (V)

(d) Current lines

Fig. 1. Normal glow regime. Conditions: 670 Pa, 293 K, $\gamma = 0.1$, $V = 2000$ V, and $R = 300$ kΩ. Cathode on the left.



(a) Ion number density (m^{-3})

(b) Electron number density (m^{-3})

(c) Potential (V)

(d) Current lines

Fig. 2. Abnormal glow regime. Conditions: 670 Pa, 293 K, $\gamma = 0.1$, $V = 2000$ V, and $R = 300$ kΩ. Cathode on the left.

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