Mathematical modelling of RF plasma flow at low pressure with electrodynamics

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Abstract. The mathematical model of the RF plasma at low pressure in both free-molecule and transition flow at Kn 0.03 ≤ Kn ≤ 3 is described. The model is based on the statistical approach for the neutral component of the plasma together with the continuum model for electron, electromagnetic field and metastable components. Results of plasma flow parameters calculations and testing results of electric field calculations are presented.

1. Introduction
RF plasma discharges at low pressures (p = 0.15 − 150 Pa) is widely used for the modification of various materials: dielectrics, conductors, and semiconductors. The plasma has the following characteristics: ionization degree is 10⁻⁷−10⁻⁵, electron density ne=10¹⁵−10¹⁹ m⁻³, electron temperature Te=1–4 eV, temperature of atoms and ions in the plasma bunch Ta=(3-4)·10³ K, in the plasma jet Ta=(3.2-10)·10² K [1-6]. One of important aspect is to investigate how the electromagnetic field influence on the plasma flow. For this purpose, equations for electric field was included with the system of equations of the plasma flow and it was made testing calculations ones.

2. Mathematical model
Hybrid model of the RF plasma is constructed, which includes kinetic model for carrier gas and continuous model for electron gas, metastable atoms and electric field. The model includes:

1) The Boltzmann’s transport equation for neutral atoms
\[ \frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} + \mathbf{F} \cdot \nabla f = S(f), \]

\[ f(c, r, 0) = f_0(c, r), \quad \mathbf{F} = -(1/m_q) \nabla \Psi \quad (1) \]

2) The equation of the electron gas continuity:
\[ \frac{\partial n_e}{\partial t} - \text{div}(D \nabla n_e - v_n n_e) = v_n n_e + R_{i+} n_e + R_{i-} n_e + R_{i^+} n_e - (R_{i-} n_e + R_{i^+} n_e) \]

\[ n_{\text{inlet}} = n_{\text{outlet}}, \quad n_{\text{inlet}} \big|_{\text{inlet}} = 0, \quad n_{\text{outlet}} = 0, \quad n_{\text{boudy}} = 0, \quad n_{\text{top}} = n_{\text{in}} \quad (2) \]

3) The equation of the electron heating:
\[ c_p \rho_e \frac{\partial T_e}{\partial t} - \text{div}(\lambda_e \nabla T_e - \frac{5}{2} k_B n_e T_e \nabla \rho_e) + \frac{3}{2} k_B \rho_e \nabla \rho_e (T_e - T_0) = \sigma E^2 - v_n n_e E_1 - I R_i n_e \quad (3) \]
\[ T_{e|\text{inlet}} = T_{e,\text{inlet}}, \quad T_{e|\text{outlet}} = T_{e,\text{room}}, \quad T_{e|\text{walls}} = T_{e,\text{room}}, \quad \frac{\partial T_e}{\partial n} = 0, \quad T_{e|\text{body}} = T_{e0}, \]

4) The equation of the metastables continuity:
\[ \frac{\partial n}{\partial t} - \text{div}(D \text{ grad } (n_e)) = R_{\text{ph}} n_e - R_{\text{n}} n_e^2 + R_{\text{a}} n_e n_n - R_{\text{a}} n_e n_{\text{a}} - R_{\text{a}} n_{\text{a}} n_{\text{n}} - R_{\text{a}} n_{\text{a}} n_{\text{n}} + R_{\text{a}} n_{\text{n}} n_{\text{a}} \quad (4) \]

5) The equation of electric fields described by the inhomogeneous wave equation known as Telegraphers equation\[7].
\[ \left( \Delta - \mu_b E_0 \frac{\partial^2}{\partial t^2} \right) E(r,t) = \mu_e \frac{\partial}{\partial t} j(r,t), \quad (5) \]

System of equation (1)-(5) is closed by the following formulae
\[ p_a = n_a k_B T_a, \quad v_a(r,t) = \int_{-\infty}^{\infty} \mathbf{f}(c, r, t) dc, \quad v_e = v_a - (D_a / n_e) \text{grad } n_e. \quad (6) \]

Here \( \mathbf{E}(r,t) \) is the electric field and \( j(r,t) \) is the current, \( \mathbf{c} \) and \( \mathbf{r} \) are vectors of velocity and coordinates of atoms, \( f/c(\mathbf{r}, r, t) \) are function of distribution of neutral atoms by velocities, \( f_0 \) is Maxwell function of distribution by velocities, \( S(f) \) is collisions integral, \( \mathbf{r} \) is force, which influence on neutral atoms in elastic collision process, \( W_T \) is energy, which transferred to atoms in elastic collision process, \( n_e \) is density of electrons, \( D_a \) is ambipolar diffusion coefficient, \( \lambda_e \) is coefficient of thermal conductivity of electron gas, \( \nu_i \) is ionization frequency, \( c_p \) is heat capacity of the electron gas, \( \nu_c \) is the frequency of elastic collisions of electrons with atoms and ions, \( \sigma \) is plasma conductivity, \( \mathbf{E} \) is the electric field vector, \( E = |\mathbf{E}|, E_i \) is ionization potential, \( k_B \) is Boltzmann constant, \( \delta = m_e / 2m_n \), \( m_a \) is atom mass, \( m_e \) is electron mass, \( R_a \) is radius of the cylindrical vacuum chamber, \( L_a \) is length, \( R_k \) is the radius of the plasma torch outlet, \( \text{subscripts } inlets, outlets, body, walls } \) are vectors of velocity and coordinates of atoms, \( f/c(\mathbf{r}, r, t) \) are function of distribution of neutral atoms by velocities, \( f_0 \) is Maxwell function of distribution by velocities, \( S(f) \) is collisions integral, \( \mathbf{r} \) is force, which influence on neutral atoms in elastic collision process, \( W_T \) is energy, which transferred to atoms in elastic collision process, \( n_e \) is density of electrons, \( D_a \) is ambipolar diffusion coefficient, \( \lambda_e \) is coefficient of thermal conductivity of electron gas, \( \nu_i \) is ionization frequency, \( c_p \) is heat capacity of the electron gas, \( \nu_c \) is the frequency of elastic collisions of electrons with atoms and ions, \( \sigma \) is plasma conductivity, \( \mathbf{E} \) is the electric field vector, \( E = |\mathbf{E}|, E_i \) is ionization potential, \( k_B \) is Boltzmann constant, \( \delta = m_e / 2m_n \), \( m_a \) is atom mass, \( m_e \) is electron mass, \( R_a \) is radius of the cylindrical vacuum chamber, \( L_a \) is length, \( R_k \) is the radius of the plasma torch outlet, \( \text{subscripts } inlets, outlets, body, walls } \) are parameter value on inlet and outlet of the chamber, on the walls of the sample, and the vacuum chamber, respectively, \( W_T = \int E_i dV dt, dV \) is volume element, \( E_c = \frac{3}{2} k_B \delta \nu_e n_e (T_e - T_0) \) is energy of elastic collisions transport.

Coefficients \( D_a, \nu_i, \lambda_e \) are functions of electron temperature \( T_e, T_i = 11.56 \text{ eV} \) is excitation energy, \( R_1 \) is impact ionization rate coefficient, \( R_2 \) is Penning ionization rate coefficient, \( R_3 \) is step ionization rate coefficient, \( R_4 \) is photo recombination rate coefficient, \( R_5 \) is triple recombination rate coefficient, \( R_6 \) is excitation of metastables rate coefficient, \( R_7 \) is radiative recombination rate coefficient, \( R_8 \) is collisional quenching rate coefficient, \( R_9 \) is electron deexcitation rate coefficient.

The plasma is quasi-neutral and therefore approach (5) is applicable. We assume that \( \mathbf{E} \) field and \( j \) current are changing harmonically in time, and can be used complex amplitude method. Given that
\[ \mathbf{E}(r) = \mathbf{E}_{\text{re}}(r) + i \mathbf{E}_{\text{im}}(r), j = \sigma \cdot \mathbf{E}(r) \quad (7) \]

we have the equations for real and the imaginary part of \( \mathbf{E} \) field:
\[ \Delta \mathbf{E}_{\text{re}}(r) = \mu_e \varepsilon_0 \omega^2 \mathbf{E}_{\text{re}}(r) + \sigma \mu_i \omega \mathbf{E}_{\text{im}}(r), \quad (8) \]
\[ \Delta \mathbf{E}_{\text{im}}(r) = \mu_e \varepsilon_0 \omega^2 \mathbf{E}_{\text{im}}(r) - \sigma \mu_i \omega \mathbf{E}_{\text{re}}(r). \]

Values of the electric fields on the boundary can be calculated using Biot-Savart law for the electric field’s vector potential:
\[ \mathbf{E}(\mathbf{r}) = -i\omega \mu_0 \int \frac{\mathbf{j}(\mathbf{s})_{\text{coil}} + \mathbf{j}(\mathbf{s})_{\text{el}}}{|\mathbf{r} - \mathbf{s}|} d^3s, \]  

(9)

where \( \mathbf{j}(\mathbf{s})_{\text{coil}} \) is current on the coil and \( \mathbf{j}(\mathbf{s})_{\text{el}} \) is current of the electrons.

3. Method of calculation and results

Bird’s method [8] is modified by introducing the spatial heat source power \( W_T \). A four-step iterative process is constructed for solving the problem (1) - (6). Equation (1) is solved by modified Bird’s method. Equations (2)-(5) is solved by finite volume method (FVM) with specified numerical scheme. Software package for finding the spatial distribution of the main plasma characteristics is developed. The package use OpenFOAM [9] library environment and works under the Linux operating system.

The gas-dynamic characteristics of low pressure RF plasma both an undisturbed jet and the jet with overflowing sample in the vacuum chamber of \( R_{vk}=0.2 \text{ m}, L_{vk}=0.5 \text{ m} \) and \( R_{gk}=0.012 \text{ m} \), on the center of the base plate is carried out. A cylindrical sample of radius \( R_b=0.03 \text{ m} \) and a height \( L_b=0.02 \text{ m} \) located in the plasma jet at a distance \( L_{tb}=0.02 \text{ m} \). Flow input parameters are the following: the plasma forming gas is argon, gas flow rate \( G=0.02–0.24 \text{ g/s} \), pressure \( P_{\text{inlet}}=3.5–135 \text{ Pa} \), the temperature \( T_{\text{inlet}}=400–600 \text{ K} \), the degree of ionization \( \delta_i=10^{-4} \). The initial pressure in the vacuum chamber \( P_0=0.35–13.5 \text{ Pa} \). Distributions of temperature, velocity, and pressure of carrier gas as well as electron temperature and density are obtained and described in previous work [10].

A model of the two-spiral coil around the tube of 0.15 m by length on position 0 cm and on 5 cm from the beginning of tube is used for testing of calculation of the equations (8). The distribution of current \( \mathbf{j} \) on each spiral on coil was set constantly 30 A/m². For calculating of \( \mathbf{E} \) field was written the program on C++ language, which uses OpenFOAM [9] library. System (8) was solved iteratively till establishing. On each iteration produced recalculating of boundary conditions on tube by relation (9) for \( \mathbf{j}(\mathbf{s})_{\text{coil}} \) and for electron volume charge current \( \mathbf{j}(\mathbf{s})_{\text{el}} \) separately. The boundary condition on the tube surface setups after summation of currents by relation (9) and iterative process continue to next step.

Figure 1 illustrates distributions of the \( \mathbf{E}_{\text{im}} \) along axis (left side) and in slice (right side). It is shown that maximum of module \( \mathbf{E}_{\text{im}} \) is on the tube boundary where it equals to 6440 V·m⁻¹, and \( \mathbf{E}_{\text{im}}=0 \) in the centre of tube. It is shown that the vector of \( \mathbf{E}_{\text{im}} \) has tangential direction. The results of calculations are quality in agree with known experimental data.
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