Mathematical modelling of RF plasma flow at low pressure with metastable and electrodynamics

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Abstract. A mathematical model of the RF plasma flow at 0.15–150 Pa, Knudsen 0.03≤Kn≤3 with metastable atoms and electrodynamics is described. The model based on both astatistical approach for the neutral component of the RF plasma and the continuum model for electron, ion components, metastable and electric field. The results of plasma flow calculations for an undisturbed jet are described.

1. Introduction
RF plasma at low pressures (0.15–150 Pa) are used for the modification of various materials: dielectrics, conductors, semiconductors [1–5]. The plasma has the following properties: ionization degree is in range from 10⁻⁷ to 10⁻⁵, electron density $n_e$ is in range from $10^{15}$ to $10^{19}$ m⁻³, the electron temperature $T_e$ is in range from 1 to 4 eV, the temperature of atoms and ions $T_a$ ranges within (3–4)×10³ K in the plasma torch and within (3.2–10)×10² K in the plasma stream, respectively. There are two features for low pressure RF plasma simulation. The first specific feature is the combination of the transient mode of the neutral component flow and the continuous medium mode of the charged component flow [6–8] due to carrier gas Knudsen parameter $Kn$ is in the range 0.03<Kn<0.8, depending on the gas consumption and pressure.

The Navier-Stokes equations are not applicable in case of neutral gas yet and certainly in plasma flow. The particle-in-cell (PIC) method is used for simulation the ICRF discharge plasma [9,10] to analyze the mechanism of power absorption in pressure range from 0.1 to 100 m Torr. Direct Monte-Carlo simulation (DSMC) is used for studying the ICRF plasma jet flow in pressure range from 0.1 to 1.0 Torr in [6–8]. The mathematical model presented in [6–8] is not self-contained, because the distribution of the electrical field strength is approximated by experimental data. The second feature of ICRF discharge is that all 6 components of the electromagnetic field must consider in common case. Therefore, the Maxwell’s equations are usually reduced to equation for vector and scalar potentials [11] or to wave equation [12], or analyzed in condition of neglecting the radial components of the magnetic field [13].

In [9, 10] the Poisson equation is used for calculation of the electric field strength. In [14] two-dimensional model of ICRF discharge in pressure range from 0.1 to 1.0 Torr is constructed with the Maxwell’s equations reduced to the system of elliptical equation for the modulus, phases and angle functions of magnetic field and electric strength vectors while the carrier gas stream is approximated by a Poiseuille flow.
Excited atoms (metastable) are essential for the balance of particles and energies in RF discharges in argon [15–19]. No data concerning the systematic study of ICRF plasma jet considering metastable in pressure range from 0.1 to 1.0 Torr can be found in modern literature. The present paper aims to construct a model of low pressure ICRF plasma to analyze a role of different particles in sustaining of the discharge. This paper deals with RF discharge without an external magnetic field in pressure range from 0.1 to 1.0 Torr.

2. Mathematical model of low pressure RF plasmas stream

As mentioned above, low pressure RF plasma flow has a transient mode between the free-molecule flow and static continuum. The Navier-Stokes equation is not correct when the Knudsen’s parameter is in range of $0.03 \leq K\nu \leq 3$ [20,21]. At the same time, both electron and ion gases satisfy continuity, since their movement is determined not only by moving with the gas flow, but also by the Coulomb force action that prevents the separation of charges [22].

Mathematical model of the low-pressure RF plasma stream is constructed by neglecting the following effects: the Hall’s effect, electron pressure gradient, the radiation energy loss, the electron attachment, the excitation of atoms, bulk recombination, formation of multiply charged ions and ions slipping. A direct electron impact as the basic mechanism of the formation of charged particles is assumed.

We also assume that the ion temperature coincides with the temperature of neutral atoms. Let the radius of the cylindrical vacuum chamber be denoted by $R_{vk}$, its length – by $L_{vk}$, the radius of the plasma torch outlet – by $R_{rk}$, the subscripts inlet, outlet, walls should be used for parameter values on inlet, outlet, and the walls of vacuum chamber, respectively.

The model in local approximation includes:

1) The Boltzmann’s transport equation for neutral atoms

$$\frac{\partial f}{\partial t} + c \cdot \frac{\partial f}{\partial x} + F \cdot \frac{\partial f}{\partial c} = S(f), \quad t > 0, \quad c \in \mathbb{R}^3,$$

$$f(c,t)_{\text{inlet}} = f(c,t)_{\text{outlet}} = f_e(c),$$

2) The equation of the electron continuity:

$$-\text{div}(D \cdot \nabla n_e + \mu_e E_{\text{cap}} n_e) = v n_e + R_{n_e} n_e + R_{n_e} n_e - R_{n_e} n_e - R_{n_e} n_e,$$

$$n_e|_{\text{inlet}} = n_e|_{\text{outlet}}, \quad n_e|_{\text{wall}} = n_e|_{\text{wall}} = 0,$$

3) The equation of the ion continuity:

$$-\text{div}(D \cdot \nabla n_i + \mu_i E_{\text{cap}} n_i) = v n_i + R_{n_i} n_i + R_{n_i} n_i - R_{n_i} n_i - R_{n_i} n_i,$$

$$n_i|_{\text{inlet}} = n_i|_{\text{outlet}}, \quad n_i|_{\text{wall}} = n_i|_{\text{wall}} = 0,$$

4) The equation of the metastables continuity:

$$-\text{div}(D \cdot \nabla (n_m)) = R_{n_m} n_m - R_{n_m} n_m - R_{n_m} n_m - R_{n_m} n_m - R_{n_m} n_m,$$

$$n_m|_{\Omega} = 0,$$

5) Poisson equation for irrotational electrical field:

$$-\Delta \phi = \frac{\varepsilon}{\varepsilon_0} (n_i - n_e), \quad E_{\text{cap}} = -\nabla \phi,$$

$$\phi|_{\text{inlet}} = \phi|_{\text{outlet}}, \quad \phi|_{\text{wall}} = \phi|_{\text{wall}} = 0,$$

6) The Maxwell’s equations for RF component of electromagnetic field in inhomogeneous wave view [23]:

$$\left(\Delta - \mu_0 \mu_e \frac{c^2}{\partial t^2}\right) E(r,t) = \mu_0 \frac{\partial}{\partial t} j(r,t),$$
\[ \mathbf{E}(\mathbf{r}) = -i\omega \frac{\mu_0}{4\pi} \int_{\Omega} \left( \mathbf{j}(\mathbf{s})_{\text{coll}} + \mathbf{j}(\mathbf{s})_{\text{el}} \right) d^3\mathbf{s}. \]

Here, \( \mathbf{c}, \mathbf{r} \) are vectors of the velocity and the coordinates of the atoms, respectively, \( f(\mathbf{c}, \mathbf{r}, t) \) is the velocity distribution function of neutral atoms, \( f_0(\mathbf{c}) \) is Maxwell’s velocity distribution function, \( S(f) \) is the collision integral, \( \mathbf{F} = -(1/m) \nabla \mathbf{W} \) is the reduced force field which effects on neutral atoms at elastic collisions with electrons, \( t \) is time, \( \Omega \) is the domain of the vacuum chamber, \( \partial \Omega \) is the boundary, which consists from inlet, outlet, and the walls of vacuum chamber, \( \mathbb{R}^3 \) is 3d Euclidean velocity space, \( n_e, n_i \) are electron and ion density, respectively, \( D_e, D_i, D_m \) are electron, ion and metastable diffusion, \( \nu_e \) is the electron collision frequency, \( \nu_i \) is the gas velocity, \( \lambda_e \) is the thermal conductivity of electrons, \( \nu_i \) is the elastic collision frequency of electrons and atoms, \( \sigma \) is the plasma conductivity, \( E_{\text{cap}} \) is strength of the irrotational electrical field, \( \mathbf{E} \) is RF electric field strength, \( E_{\text{full}} = E + E_{\text{cap}}, E = |E_{\text{full}}|, dV \) is elementary volume, \( R_1 \) is impact ionization rate, \( R_2 \) is Penning ionization rate, \( R_3 \) is step ionization rate, \( R_4 \) is photorecombination rate, \( R_5 \) is triple recombination rate, \( R_6 \) is excitation of metastable rate, \( R_7 \) is radiative recombination rate, \( R_8 \) is collisional quenching rate, \( R_9 \) is electron deexcitation rate, \( \mathbf{j}(\mathbf{s})_{\text{coll}} \) is current on the coil and \( \mathbf{j}(\mathbf{s})_{\text{el}} \) is electron current in plasma.

Coefficients \( D_e, D_i, D_m, \nu_e, \nu_i, \mu_e, \mu_i \) are functions of the reduced electric field \( (E/N) \), where \( N \) is density of neutral particles [24, 25]. Rates \( R_k, k = 1−9 \) are described in [8, 26–34]. The boundary conditions for equation (6) sets from the Biot-Savart law.

The direct statistical Monte-Carlo (DSMC) modeling [35–38] is widely used for the numerical solution of problems of the rarefied gas dynamics. The method is based on the splitting of the Boltzmann’s equation on the movement and collision processes that allows us to describe the gas-dynamic processes in the transition mode for neutral environment. Therefore, both modification of the Bird’s method for calculation of rarefied RF plasma flows and bringing it in compliance and fitting with the continuous model of charged particles are required. The software package using libraries of OpenFoam open source CFD software [39] was created for calculations the plasma parameters.

3. Results of numerical experiments

The calculations of main parameters of RF plasma in vacuum chamber for neutral component, charged component and electromagnetic field was performed.

The radius of cylindrical vacuum chamber \( R_{vk} \) is 0.2 m, length \( L_{vk} \) is 0.5 m and radius of input hole \( R_{gk} \) is 0.012 m. The plasma gas is argon, flow rate \( G = 0.02−0.24 \text{ g/s} \), inlet pressure 0.15−150 Pa, the temperature is from 400 to 600 K. The initial pressure in the chamber is 0.015−15 Pa, the electrical potential \( \phi_{\text{inlet}} \) is -1000 V, the initial vortex field on the inlet is in range of 500–1500 V/m.
Pressure profiles is bell-shaped in cross-section of the undisturbed jet such as in [8]. The velocity profile of the neutral gas also is a bell-shaped in cross-section of undisturbed flow and monotonically decrease along the Oz-axis.

The temperature profile of the neutral gas is a bell-shaped in cross-section of plasma jet and monotonically decrease along the Oz-axis, except small zone near the inlet due to jet spreading and pressure decreasing, figure 1(a).

The potential of electrical field has maximum at $z = 0.08$ m on the jet axis and decrease in direction to vacuum chamber walls, figure 1(b). Thus, the RF plasma jet is an electrode positively charged against the walls. The RF electrical field is axisymmetric and directs to vacuum chamber walls. The irrotational electrical field is non-symmetric in accordance to formulae (6). It is directed to walls at $x < x_{\text{max}}$, $y < y_{\text{max}}$, $z < z_{\text{max}}$ where $(x_{\text{max}}, y_{\text{max}}, z_{\text{max}})$ is the point of $\max(\phi(x,y,z))$, and from the walls to Oz-axis at $x > x_{\text{max}}$, $y > y_{\text{max}}$, $z > z_{\text{max}}$. Asymmetry in distribution of $E_{\text{cap}}$ disturbs the symmetry of electrical field near the Oz-axis, figure 2. The maximum value of the modulus of tension of the full electric field is achieved at the inlet chamber and equals to 5000 V·m$^{-1}$. Density of the charged particles is a bell-shaped in jet cross-sections. Maximum concentrations are achieved at the inlet.
4. Conclusions
The mathematical model of the RF plasma flow at pressure of 0.15–150 Pa with metastable atoms and electric field is developed. Results of plasma flow calculations for charged particles and metastable density, neutral component velocity, pressure and temperature, electrical field are described. It is established that the electrical field is asymmetric about Oz-axis due to asymmetry of irrotational component of the field. The electrical potential is reached the maximum value on the jet axis and is positive about the walls. The temperature distribution of neutral plasma component is decreased near the inlet and is bell-shaped in jet cross-section in the remaining part.

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